IB Chemistry IA Handbook

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(For use with the IB Diploma Programme)

(Fourth edition)

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Published by IBID Press, Victoria, Australia

Third Edition 2014

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Library Catalogue

1. Chemistry
2. International Baccalaureate Chemistry Diploma Programme.
3. Internal Assessment Handbook
4. Talbot C

ISBN: 978-0-9925224-3-8

Published by IBID Press, 36 Quail Crescent, Melton 3337, Victoria, Australia.

Samples of other materials to support the teaching of IBO syllabuses can be found at: www.ibid.com.au

Foreword

This 'Student Handbook for Internal Assessment - Chemistry' has been written specifically to support the teaching of the current International Baccalaureate Chemistry course (© International Baccalaureate Organisation 2014). It has been written by an experienced and practising Senior Chemistry Teacher with close reference to the Group 4 Internal Assessment criteria.

The material was written with close reference to the IBO Diploma Programme Chemistry Guide published in March 2014. Some material is reproduced from the Guide and other material is adapted from the Guide. *The assessment criteria have been divided into sections and sub-sections, but this division has been implemented by the author and is not mandated by the IBO.*

This material has been designed to accompany and complement Chemistry for use with the International Baccalaureate (4th edition) written by Dr John Green and Dr Sadru Damji and published by IBID Press, and the three Volumes of Investigations for IB Chemistry written by Dr John Green and published by IBID Press. It will, however, be useful to IB Chemistry students following any practical scheme of work and using any published text book.

The aim of this Student Handbook is to help you, as an IB Physics student, to plan conduct and write a report for an Individual Investigation for Assessment and conduct and write a report for other practicals or investigations including your Group 4 Project as required by your teacher. It contains a wide variety of information and advice that will help you at various stages throughout your IB Chemistry practical programme including the completion of your Individual Investigation. A separate chapter is included for students who are studying chemistry for their Extended Essay.

The Guiding Questions (inspired by the IB MYP approach) have been written by the Author and the Editor and are designed to help you consider the important concepts and understandings inherent in the group 4 assessment criteria. The guiding questions are generative, meaning they generate multiple avenues of inquiry and investigation as you plan, perform and write-up your Individual Investigation. Active questioning will keep your brain engaged: an inquiring mind is absorbing information and constructing meaning. Deliberate and thoughtful questioning involves higher order thinking skills and depth of knowledge.

Both Standard and Higher Level IB Chemistry students should find this Student Guide useful. It includes material that will be relevant to students of all linguistic and academic abilities. Although the author is European, he has consulted a North American colleague to ensure that the conventions are also recognisable and relevant to American and Canadian students.

Christopher Talbot (Author)

Singapore 2014

Internal Assessment

The individual assessment allows students to develop and demonstrate their skills in scientific research.

The initial planning is vital to the success of the individual investigation. Students will be guided by the teacher as to the appropriateness of the research question – level of complexity and compatibility with the assessment criteria.

The individual investigation is personal research and each student will undertake a unique investigation of a Research Question that is of interest. The formulation of the research question is the responsibility of the individual student.

Each student should decide whether the investigation is a hands on investigation or uses secondary sources such as databases. A mix of various types of investigation is allowed.

1. There is no expectation to go beyond content of the syllabus. Work can be based on concepts within the course specifications.
2. One **investigation** is required and it must be individual work - no partners or sharing of data.
3. The assessment model uses five criteria to assess the final report of the investigation with the following raw marks and weightings assigned (*refer to the IBO Syllabus Guide*).
4. Levels of performance are described using multiple indicators per level. Also, not all indicators are always present. It very much depends upon the type of investigation.
5. The **investigation** should take about 10 hours of work.
6. There will be a **single investigation** by the student and the report can be **6 to 12 pages long**, have an academic and scholarly presentation, and demonstrate scientific rigor commensurate with the course.

The IA combines research and experimental work.

Author Profile

Chris taught IB Chemistry, IB Biology and Theory of Knowledge (ToK) in the High School of the Overseas Family School, Republic of Singapore. He now teaches at a leading IB World School in Singapore. He graduated with Honours in Biochemistry from the School of Biological Sciences, University of Sussex in the United Kingdom. He also holds an Advanced Certificate in Molecular Biology from Birbeck College, University of London in the United Kingdom. He has a Masters degree in Life Sciences (Chemistry) from the National Technological University (NTU) in Singapore. He is the co-author of the MYP Student Guide and MYP Practical Portfolio and the author of the Practice Examinations for IB Chemistry and IB Biology. He is a contributing author to the fourth edition of the IB Biology text book published by IBID Press. He has had many Chemistry and Biology articles published in '*School Science Review*' and is serving a five year term as an Editorial Associate.

Acknowledgements

It is a considerable pleasure to acknowledge the extensive advice and numerous contributions of the following during the production of the fourth edition: Cesar Reyes (Overseas Family School) and Dr John Green (formerly of Li Po Chun United World College).

The author, editor and publisher acknowledge and appreciate permission given by the IBO to use and adapt material from the Syllabus Guide.

Any mistakes and omissions remain the responsibility of the author. Feedback and comments relating to this publication may be sent to the Publisher. The author welcomes constructive feedback (via the publisher) from both students and teachers on the current contents and suggestions for inclusions in future editions.

The Individual Investigation

In the second year of the IB Diploma programme you will be required to research, design, perform (carry out) and write-up your own Individual Investigation. The internal assessment (IA) accounts for 20% of your final IB Diploma grade for IB Chemistry and requires you to spend 10 hours performing laboratory work, during which time you will be in communication with your teacher who will act as your supervisor. The time required for you to write the report for your own Individual Investigation cannot be included in the 10 hours and this should be done outside of the laboratory period.

A range of possible types of investigations can be carried out for the Individual Investigation.

You will probably be encouraged by your Chemistry Teacher to carry out traditional hands-on experimental work. For example, you may want to synthesize and purify aspirin and analyse it using a variety of chemical techniques including a back titration and spectroscopic techniques.

You may also go on-line and retrieve data from a reliable chemical web site and process, analyse and present the data for your own analysis and investigation. Some aspect of atmospheric or environmental chemistry may be suitable for this type of Individual Investigation.

You may use of a spreadsheet to set up a model to simulate some physical chemistry phenomenon, for example, chemical equilibrium, kinetics or a pH curve. You can compare the theoretical data against experimental data and evaluate the experimental data and any assumptions in your model.

In actual practice some combinations of some or all of these approaches may be suitable, depending on the topic of the Individual Investigation.

The subject matter or content may be inside or outside the current of the IB chemistry syllabus. The subject matter of your Individual Investigation is your decision, as the student, but you must ensure you are familiar with any new chemical facts, principles and concepts. However, your knowledge of IB chemistry (SL or HL) will enable you to get the maximum mark when the write-up of your Individual Report is assessed by the IBO.

The Individual Investigation (your Internal Assessment (IA)) will consist of a report 6 to 12 pages long. The report should resemble a scientific paper from the chemical literature. It should be an academic piece of work and show the scientific rigour expected from a SL or HL chemistry student. You are expected to show a high degree of personal involvement and a good scientific understanding of the chemistry that lies behind your Individual Investigation. It is important that your summarize the current chemical thinking and knowledge of your chosen topic.

Health and Safety Symbols

Laboratories can be hazardous places. Often scientists, Science teachers and students handle equipment and materials which can be dangerous to their health and safety. In this series of Volumes you will see a number of symbols and warnings which will represent particular hazards. For each of these we will briefly describe the hazard and indicate what precautions you should take to avoid damage and/or what responses are appropriate. In all cases, of course, you should seek advice and assistance from the teacher or laboratory technician.

A biohazard is any organism or body fluid which could possibly cause illness or disease in your body. This particularly includes micro-organisms.

A flammable substance is one which will readily burn in air. It may be a solid, liquid or gas. If you are using such a substance it is vital that there are no sparks or naked flames which could ignite it. It is vital that you know what to do in the event of fire. This may include the use of fire extinguishers and evacuation procedures.

A radioactive substance is one which emits particles or 'radiation'. This radiation is known to cause damage to cells and may also be cancer causing. If you are using radioactive substances it is vital that you wear protective clothing, use metal tongs and listen carefully to instructions given by your teacher or laboratory technician.

Sharp instruments are often used in Science and particularly in Biology, to cut sections through plant or animal tissue. These instruments, which include scalpels and razor blades are very sharp and obviously will also cut through your tissues. When using these instruments it is essential that you always cut away from your body and preferably onto a cutting board. It is also important to be very careful when carrying these instruments and also ensure they are placed on the workbench in a safe place.

When certain chemicals are mixed together they can become explosive. An explosion is caused by rapid expansion of gas in a confined space and can be very dangerous. Sometimes it is important to ensure that the space is not confined and sometimes it is important to conduct these reactions behind a protective screen.

It is often necessary to protect your hands from heat, chemicals or other hazards and gloves will be made available for these situations. The type of glove needed will depend on the particular hazard and your teacher will provide further advice. In some cases you will be advised to dispose of the gloves after use and in other cases to wash and dry them carefully.

Your eyes are the most vulnerable and easily damaged external part of your body. This is why they must be protected if you are using solids and liquids which could get into them. Whenever you are heating things or using corrosive liquids, and in other cases as instructed by a teacher, you should wear safety goggles. You should also do this if possible even if you wear spectacles to correct your vision. In the event that something gets in your eye you should immediately make use of the eyewash facility in the laboratory as instructed and then notify your teacher.

Some chemicals, which are used in a laboratory, are *corrosive*. This means that they can react with and 'eat away' materials like the bench, your books, clothing and skin. It is essential that you handle these materials, which are usually liquids, with care. Always tip from the container with the label uppermost, never add water to concentrated acid and never have your face anywhere near the container. It is usually advisable to wear both safety goggles and gloves. If protective aprons are available you should also wear one.

As a general rule, 12 or 24 volt *electrical* appliances are unlikely to cause serious injury. However, 'mains' voltage (110V or 240V or higher) can cause serious injury or death. The appliances you use should be regularly tested and certified safe. If you notice sparks or smell insulation burning, turn the power off immediately and notify staff. Be particularly careful not to allow water to get into any appliance as it may cause a short circuit.

Some chemicals are *poisonous* and should not be inhaled or ingested. It will be necessary to use a fume cupboard when using poisonous gases or volatile liquids. They could make you very ill and you may require medical assistance. It is vital that you listen to instructions, follow them carefully and notify your teacher immediately if there is accidental exposure to poisonous or toxic substances.

Lasers are very intense beams of light. They are capable of causing burns to the skin and permanent damage to the eyes. It is essential that these are only ever used under the supervision of a teacher and in a situation where people can not see the beam directly or when it is reflected from a shiny surface. Sunglasses or welding masks do not provide sufficient protection and special 'laser glasses' must be used where there is a risk.

UV light is harmful to skin and especially eyes. Do not expose these areas directly to a UV light source. If it is not avoidable, sunscreen can be applied to the skin and special goggles should be worn.

There are other *dangers* or hazards as well, for example carrying heavy or hot objects. This may also include chemicals which are not poisonous but which may smell unpleasant or irritate the skin. Whenever you see this icon more information will be provided in the adjacent text about the specific danger.

In Science and particularly in Biology, there are situations when ethics and ethical issues need to be considered in experimental work. This is particularly the case when human volunteers are being used, not just for experimental work but also when they are being surveyed to collect personal information. In these cases a consent form should be used to explain the nature of their involvement and to get their approval. Ethics will also be an issue whenever animals are used in experimentation or when they are collected in the field. They should not be exposed to conditions that are outside their natural range of tolerance and wild animals must be released back where they were sampled with the minimum of disturbance.

The environment and environmental issues become important when hazardous substances are used or produced during an experiment. Their disposal must result in minimal impact on the environment. In field work the protocol that is used must reflect practices that minimise the impact of the investigation on the site.

IMPORTANT NOTE

Although every care has been taken in preparing and trialling these investigations, absolutely no responsibility or liability whatsoever can be accepted for any damage or accident which may occur for whatever reason during the conduct of any of these activities. The Safety Warnings and Icons are advisory only and are not intended to be exhaustive or exclusive. It is a strict condition of sale that safety in the laboratory is the responsibility of the staff and students doing the laboratory work and not the author, editor or publisher of this work.

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This criterion assesses the extent to which the student engages with the exploration and makes it their own. Personal engagement may be recognized in different attributes and skills. These could include addressing personal interests or showing evidence of independent thinking, creativity or initiative in the designing, implementation or presentation of the investigation.

MARK	DESCRIPTOR
0	The student's report does not reach a standard described by the descriptors below.
1	**The evidence of personal engagement with the exploration is limited with little independent thinking, initiative or creativity.** The justification given for choosing the research question and/or the topic under investigation does not demonstrate **personal significance, interest or curiosity.** There is little evidence of **personal input and initiative** in the designing, implementation or presentation of the investigation.
2	**The evidence of personal engagement with the exploration is clear with significant independent thinking, initiative or creativity.** The justification given for choosing the research question and/or the topic under investigation demonstrates **personal significance, interest or curiosity.** There is evidence of **personal input and initiative** in the designing, implementation or presentation of the investigation.

The following Guiding Questions may be helpful:

- ***To what extent does the report show evidence of independent thinking, initiative or creativity?***
- ***To what extent has the student justified a research question that shows personal significance, interest or curiosity?***
- ***What evidence is there of personal input and initiative in designing, carrying out and presentation of the investigation?***

Your mark for personal engagement will be judged from the written evidence and is based on the your individual work on the Individual Investigation. Your teacher will take into account your self motivation and perseverance that is evidenced in the report for the Individual Investigation.

To score maximum marks under the personal engagement criterion you must provide clear written evidence and evidence to your teacher that you have contributed significant scientific thinking, initiative, or insight into your Individual Investigation. You should take 'ownership' of the Individual Investigation and show all the traits and characteristics of a research student.

Your research question could be based upon some theory covered in class, for example, pollution of water by antibiotics, or an extension of your own personal interest, for example, medicinal chemistry, which you may be intending to study for a degree at University. You may have prepared and analysed aspirin in class, but you are interested in synthesizing and analyzing paracetamol.

Your teacher may have shown an interesting demonstration that captured your interest. For example, the production of 'slime' (*Figure 101*) resulting from the cross-linking of polyvinyl alcohol (PVA).

<http://www.cmu.edu/gelfand/k12-teachers/polymers/polymer-architecture/polyvinyl-alcohol-slime.html>

Figure 101 Polyvinyl alcohol 'slime'

If you have strong mathematical skills you may want to construct a spreadsheet simulation for an oscillating chemical reaction demonstration. You may have watched a video or read about the discovery of carbon-60 (*Figure 102*) and want to construct your own carbon-60 generator by electrically burning graphite rods in a helium atmosphere inside a bell jar.

<http://en.wikipedia.org/wiki/Fullerene#mediaviewer/File:C60_Fullerene_solution.jpg>

You may have a closer personal involvement, for example, you may have limited night vision and be interested in studying the anti-oxidant properties of carotene in carrots. You may have lived in a country and observed the effects of a particular form of pollution, such as acid rain or heavy metal pollution.

Figure 102 Carbon-60 dissolved in an organic solvent (methylbenzene)

If you are a school athlete you may be personally interested in the effects of illegal drugs, such as anabolic steroids, and their detection. You may want to use instrumentation available at a research laboratory or university.

You can demonstrate personal engagement via personal input and initiative in the design (planning), implementation (carrying out), or presentation (write-up or report) of the Individual Investigation. Perhaps you taught yourself the principles of retrosynthesis and were able to dissect a commercial drug molecule and design a synthesis, or investigated the side products formed during the synthesis of simpler drugs.

Personal engagement is intended to be a way of crediting your originality in application and design. Superficial investigations or unmodified and unjustified standard methods from chemistry text books would score poorly in this criterion. Your method should not simply be a 'recipe' where you follow a standard technique with no comment, no justification and no modification.

You are more likely to score highly in this criterion if you designed and built your own apparatus. These may include a polarimeter (*Figure 103*) (for investigating optical activity) or apparatus for investigating paramagnetism, ion exchange column or paper electrophoresis.

Your self motivation towards the Individual Investigation will be formally assessed by your Teacher. This means that written work involved must always be handed in on time and complete. You may also be assessed on the issues of plagiarism. This could involve copying someone else's investigation design or conclusion and evaluation. It could also involve using someone else's processed data from their Individual Investigation or copying their calculations.

You will also be assessed on whether you approach your Individual Investigation with integrity. This could involve making up results to fit a preconceived relationship or hypothesis, ignoring results which are unexpected (anomalous data) or not acknowledging if you obtained some of your raw data in a book or from the Internet.

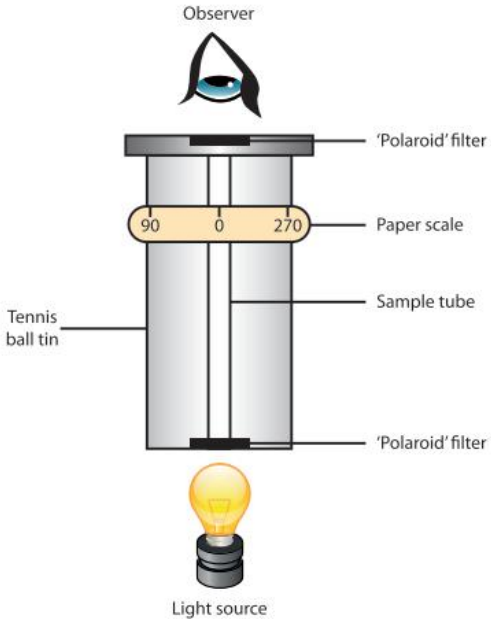

Figure 103 A simple home-made polarimeter

Exercises

Imagine you are going to investigate the effect of crab chitin on the adsorption of heavy metal ions.

- Do some research and find out about this as a technique for purifying water and justify its possible significance to an IB student.
- Is it a viable Individual Investigation?
- What methodology could be used?
- Can it be performed in a school laboratory?
- Could other biological materials, for example, hair, be used to adsorb metal ions from solution?

(N.B. No answers are provided to any of the Exercises in this Handbook)

Listed in Figure 104 is a summary of what you need to do to score well in the Personal Engagement criterion.

Assessment criteria	Evidence required	What you must do
The evidence of personal engagement with the exploration is clear with significant independent thinking, initiative or creativity.	A justified research question	You must justify the choice of research question and the chemical topic under investigation and demonstrate personal significance, interest or intellectual curiosity.
	Personal engagement during the exploration	You show significant independent thinking, initiative or creativity in the report (write-up) of your Individual Investigation, especially in the introduction. Your work must be original.
	Personal engagement during, before and after the exploration	You show personal input and initiative in the design, implementation or presentation of the investigation. Any reflective modifications to the method should be outlined and justified.

Figure 104 Summary of the Personal Engagement criterion

This criterion assesses the extent to which the student establishes the scientific context for the work, states a clear and focused Research Question and uses concepts and techniques appropriate to Diploma level. Where appropriate, this criterion also assesses awareness of safety, environmental, and ethical considerations. The following table is an extract from the IB Chemistry Guide and is the basis that will be used by your teacher and the moderator for the assessment of your work.

MARK	DESCRIPTOR
0	The student's report does not reach a standard described by the descriptors below.
1-2	The topic of the investigation is identified and a Research Question of some relevance is stated but it is not focussed. The background information provided for the investigation is superficial or of limited relevance and does not aid the understanding of the context of the investigation. The methodology of the investigation is only appropriate to address the Research Question to a very limited extent since it takes into consideration few of the significant factors that may influence the relevance, reliability and sufficiency of the collected data. The report shows evidence of limited awareness of the significant safety, ethical or environmental issues that are relevant to the methodology of the investigation *
3-4	The topic of the investigation is identified and a relevant but not fully focused Research Question is described. The background information provided for the investigation is mainly appropriate and relevant and aids the understanding of the context of the investigation. The methodology of the investigation is mainly appropriate to address the Research Question but has limitations since it takes into consideration only some of the significant factors that may influence the relevance, reliability and sufficiency of the collected data. The report shows evidence of some awareness of the significant safety, ethical or environmental issues that are relevant to the methodology of the investigation*.
5-6	The topic of the investigation is identified and a relevant and fully focused Research Question is clearly described. The background information provided for the investigation is entirely appropriate and relevant and enhances the understanding of the context of the investigation. The methodology of the investigation is highly appropriate to address the Research Question because it takes into consideration all, or nearly all, of the significant factors that may influence the relevance, reliability and sufficiency of the collected data. The report shows evidence of full awareness of the significant safety, ethical or environmental issues that are relevant to the methodology of the investigation.*

Guiding questions:

- ***To what extent does the choice of investigation allow for concepts and techniques appropriate to Diploma level to be employed?***
- ***To what extent has the student stated a clear and focused Research Question?***

2.1 The Research Question

2.1.1 Choosing a topic

Introduction

The Individual Investigation seeks to develop the IB candidate's investigative skills and to provide opportunities for self-motivation, independent learning and the planning and designing of appropriate experiments. It also provides the candidate with an opportunity to write in a scientific manner which reveals the significance of the findings of the Individual Investigation by analysing and interpreting the results in a critical and scientific manner and demonstrating knowledge and understanding of the chemical basis of the Individual Investigation.

The Individual Investigation is assessed internally through the five Group 4 Assessment Criteria and moderated externally by the IBO (if sampled). The length of the Individual Investigation work is 10 hours and this includes the planning stage and the experimental work. After completion of the Individual Investigation, the Report for the assessment is likely to take a further 5-10 hours.

It is likely that consultation with your Chemistry Teacher will ensure an early focus and clear direction as to the suitability of the topic chosen for your Individual Investigation. While you will be involved in initial reading and research, it is important that this aspect of the Investigation does not take too much time of your time.

You should consult a wide variety of sources in selecting topics for investigation. The sources that might be consulted could include: Chemistry text books and practical books, journals and periodicals, e.g., *New Scientist, Chemistry Review* (published by Philip Allan) (especially its project pages section), The *Australian Journal of Education in Chemistry, Journal of Chemical Education, Education in Chemistry* and *School Science Review* published by the ASE (print and on-line) and Internet web sites.

Focused investigations completed in the time available are likely to be the most successful. Well-controlled investigations will score higher marks than investigations with too many input variables from which valid conclusions cannot be drawn. A good investigation will generate a variety of raw data that can be manipulated via calculations and presented by graphs.

Time constraints, chemical laboratory facilities, availability of chemical equipment/apparatus, chemicals, costs and safety are all factors that need to be considered when you choose investigation topics.

While your chemistry teacher should encourage you to be creative and original, the Individual Investigation does not require it to be a piece of original research but should be new to you as an IB Chemistry candidate.

Examples of investigation topics

Let us consider chemical kinetics as topic to select a reaction as an Individual Investigation. You may have carried out practicals involving studying the reaction between calcium carbonate and hydrochloric acid. You may have investigated the effect of surface area of the calcium carbonate, or the temperature or concentration of the acid. This practical is unlikely to score high marks as an Individual Investigation.

A more suitable reaction for a kinetic study might be a more complex reaction investigated by a method not specified in the IB Chemistry syllabus. For example, the *Harcourt Essen* reaction. First find the order of reaction with respect to hydrogen peroxide, iodide and acid using a 'clock' reaction.

Therefore you could find the rate equation, rate constant and suggest a possible mechanism. Then find the order of reaction with respect to catalyst, or look at the effect of catalyst on order of reaction of hydrogen peroxide or find the activation energy with and without catalyst.

Another 'clock' reaction is the reaction between iodide and persulfate ions. First find the order with respect to iodide and persulfate using a 'clock' reaction. Therefore find the rate equation, rate constant and suggest a possible mechanism. Then find the activation enthalpy, or look at the effect of ionic strength or explore the effect of d-block ion catalysts.

A suitable Individual Investigation may take you beyond the IB Chemistry syllabus and build on your strengths in mathematics, for example, investigating the *Freundlich* adsorption isotherm from surface chemistry which is a curve relating the concentration of a solute on the surface of an adsorbent to the concentration of the solute in the liquid with which it is in contact.

You could shake different concentrations of ethanoic acid with activated charcoal, filter and find the concentration of acid remaining in solution by titration with sodium hydroxide solution. Use the data to calculate the *Freundlich* constants and extend to other acids such as methanoic, propanoic and ethanedioic acids.

The IB Learner Profile encourages diploma students to be 'risk takers' and a suitable Individual Investigation may involve growing crystals via precipitation in a sodium silicate gel. This is a diffusion technique and it is often found that crystals grow in banded arrangements known as Liesegang Rings (*Figure 201*). The formation of these rings has not been fully explained and a number of variables can be investigated, for example, pH and the passage of an electric current (AC or DC.). *Figure 201* is taken from <*http://en.wikipedia.org/wiki/Liesegang_rings* >

Figure 201 Liesegang Rings

2.1.2 Characteristics of a good Research Question

A Research Question is a focused and challenging question addressing a chemical problem or controversy with the aim of answering it by a conclusion that is based on the analysis and interpretation of chemical data.

The Research Question is a critical component of the investigation. When the aims of your study are clearly defined, this helps determine all other aspects of your investigation. The Research Question dictates the whole process; it drives your investigation design including how data are to be collected and processed and what evidence is required. It guides your analysis and interpretation of the processed data and the chemical arguments associated with them.

Hence, the Research Question can certainly make or 'break' your Individual Investigation. If your Research Question is weak, it would be too difficult to compensate for it in the other aspects of the study; and the whole investigative process is unlikely to be successful. Remember, a question well asked can lead to a question well answered.

Therefore, a good Research Question is at the heart of a great investigation. At the IB Diploma level, it is expected that the Research Question has a narrow focus and yet, it allows for an extensive exploration of the topic appropriate to Diploma level, given the available time, resources and ethical constraints.

A Research Question is deemed appropriate to IB Diploma level when it has the following characteristics:

- The Research Question encourages a complex answer. It is not answerable by a simple 'yes or no.' The answer to it should not be immediately obvious. It should have multiple possible answers and it is capable of generating multiple insights and possible surprises. The Research Question that aims to verify a known principle or physical or chemical law is unacceptable, as the answer to it is already known.
- The Research Question is amenable to the formulation of a testable hypothesis. It is grounded on a theoretical chemical framework and has the potential to lead to a meaningful investigation design and methodology.
- The answer to the Research Question transcends the raw data. It is expected that the analysis and interpretation implemented to answer the Research Question go beyond the raw data. It involves variables that can be determined from the raw data and includes cause and effect relationships. It allows for a reasonable amount of data processing that shall include some calculations and graphing of processed chemical data (not just raw data) and a meaningful interpretation of the graphs (including gradients and intercepts) and tables.
- The Research Question takes ethical and safety issues into consideration. You need to carry out a risk assessment but you need to strike a balance. You must be aware of any toxic reagents you are using and suggest suitable safe practices. But there is no need to list putting on gloves, lab coat and safety glasses or goggles at every stage of the investigation.
- Equally important, the Research Question must be communicated effectively, that is, the Research Question is well written and well phrased. It is both clear and concise. It identifies both the independent and dependent variables, and where appropriate, the controlled variables and possibly the method.

It uses simple language and includes scientific terms only when they add meaning to the statement. It is such a disservice to your study if you have an interesting investigation but your Research Question was stated inadequately.

For example, you may be investigating the growth processes, for example, tube formation, (and a variable that may control it) that occurs during the formation of a 'crystal garden'. Chemical gardens are obtained from the precipitation reaction on adding crystals of soluble metal salts to an aqueous solution of sodium silicate or introducing sodium silicate into a solution of a transition metal salt.

However, almost a hundred years later, and several centuries on from the first observations of so-called metallic trees by the early chemists such as *Glauber,* crystal gardens remain incompletely understood.

Hence to write your Research Question, 'Investigating a Crystal garden' is insufficient and does not reveal the complexity of the investigation.

2.1.3 Examples of unsuitable and suitable Research Questions

Shown below are some examples of how to formulate and write the Research Question.

Example 1 (Unsuitable)

How does temperature affect the solubility of potassium chloride?

This is a simplistic Research Question and probably not suitable for an Individual Investigation, though it may be suitable as a simple practice exercise. It is unfocussed because the solvent is not specified. It may be helpful to include the units for solubility in the Research Question. This Research Question does not offer the possibility of employment of concepts and techniques appropriate to Diploma level. Little data processing may be generated from the practical work.

Example 2 (Unsuitable)

To investigate rusting of iron

This Research Question is unfocussed. Are you trying to find out the chemical nature of rust? Are you trying to find out which substances in the air are involved in rust formation? Here is a more focused Research Question:

What is the effect of the concentration of dissolved sodium chloride solution on the rate of rusting of iron nails as measured by their increase in mass?

Example 3 (Suitable)

What is the relationship between the concentration of nitric acid (at constant temperature) and the rate of reaction between hydrogen ions (hydrochloric acid) and thiosulfate ions (sodium thiosulfate) as measured by the time taken for a sulfur precipitate to obscure a cross under the flask?

This is a very focused Research Question that identifies the independent and dependent variables as well as the method and controlled variables.

Example 4 (Suitable)

What is the relationship between the temperature and the rate of reaction between magnesium and excess hydrochloric acid as measured by the volume of gas collected per second with a gas syringe?

This is a very focused Research Question that identifies the independent and dependent variables as well as the method and units of rate.

Exercise

Write suitable focused Research Questions for examples 1 and 2.

2.2 The Investigation In Context

Guiding questions:

- ***To what extent has the student established the scientific context for the work through a discussion of its significance?***
- ***How well has the student justified their choice of Research Question and approach to the investigation?***

2.2.1 Justification for the investigation

The Research Question can be put into context by:

- **stating** why this is an important question to be answered and/or why you found this to be a particularly interesting question. A question is worth investigating if it is unresolved or unanswered by existing chemical literature. Your methodology may also be an innovative process to find supporting data or falsify an existing hypothesis.
- **discussing** the background material that is particularly relevant to the Research Question and by summarising the current understanding of the problem you are investigating.
- **addressing** how your investigation will help to fill in the holes in our current chemical knowledge of the topic.

Scientific hypotheses are testable hypotheses. This means that you need to be able to perform an experiment and take measurements and formulate hypotheses to establish how two variables are related.

- A good hypothesis states an expected relationship between the dependent and independent variables and clearly explains or justifies the relationship between variables.
- A good hypothesis reflects the theory or literature on which they are based. A good hypothesis has a substantive link to existing chemical literature and chemical theory.
- The Exploration criterion does not explicitly require a hypothesis but formulating one can help you give direction to your investigation and form an important part of the background of your planning and report. Formulating a hypothesis requires you to state clearly what you intend to change and measure. This is crucial as it can lead you to a reasonable experimental design.
- The ultimate value of the hypothesis is that its explanation, if linked convincingly to existing theory and literature, can give you the opportunity to demonstrate higher level order thinking skills necessary to access the assessment criteria at a higher achievement level.

2.2.2 Writing the background from the literature

A review of the chemical literature related to your Individual Investigation has the following functions:

- To justify your choice of Research Question, theoretical or conceptual framework, and method.
- To establish the importance of the chemical topic.
- To provide background information needed to understand the study.
- To show your IA Assessor you are familiar with significant and/or up-to-date research relevant to the topic.
- To establish your study as one link in a chain of research that is developing knowledge in this field of chemistry.

The review will provides a historical overview of the theory and the research literature, with a special emphasis on the literature specific to the Individual Investigation topic. It serves as well to support the argument/proposition behind your thesis, using evidence drawn from authorities or experts in your research field.

For example you may have chosen to study an oscillating reaction such as the *Belousov* and *Zhabotinskii* (BZ) reaction for your Individual Investigation. A literature search will reveal that the study of non-linear reactions began in 1968. At a conference in Prague that year, the work of *Belousov* and *Zhabotinskii* on oscillating chemical reactions, done in Moscow in the fifties and early sixties, became widely known to Western scientists. The field of oscillating reactions received a further boost in 1972, when *Noyes* at the University of Oregon suggested a chemical mechanism for the

Belousov-Zhabotinskii reaction. In the mid-seventies, a French research group pioneered the use of the continuous-flow stirred tank reactor for the study of chemical oscillations and chaos. One importance of oscillating reactions is their possible connection to pattern formation in embryos.

However, it is important that you do not include any advanced material that is not directly relevant to the Individual Investigation or you do not understand and explain clearly.

2.2.3 Formulating the hypothesis

In chemistry, a hypothesis is a prediction and associated explanation of the type of chemical behaviour or result expected during a chemical investigation. Hypotheses enable the design of investigations so that predictions based upon a hypothesis may be tested and either tentatively 'supported' or 'disproved'. Many IB Chemistry investigations will start with a hypothesis or a pair of competing hypotheses. They should be supported by a detailed justification using relevant chemical concepts (especially those at the ionic, atomic or molecular level).

The IB Learner Profile encourages IB students to be 'risk takers' and this can be interpreted as encouraging you to investigate physical relationships not included in the IB Programme, for example, to establish whether there is a relationship between the strength of an acid (as measured by its acid dissociation constant, K_a) and its enthalpy change of neutralization.

Examples of hypotheses

Introduction

Hypotheses may be qualitative, for example, an increase in temperature will increase the rate of reaction between zinc granules and dilute aqueous hydrochloric acid. This behaviour is accounted for by the increase in collision rate between zinc atoms (on the surface of the zinc) and hydrogen ions (in aqueous solution) and, more importantly, the increase in the fraction of collisions between these species that have combined kinetic energies greater than, or equal to, the activation energy.

Where possible, the hypothesis should be quantitative, and describe the relationship between a dependent and independent variable. For example, every rise of ten degrees Celsius will double the rate of reaction between zinc and dilute aqueous hydrochloric acid.

Arrhenius temperature dependence

This is known as Arrhenius temperature dependence and a detailed quantitative 'proof' of this behaviour using the principles of kinetic theory is shown below.

We need to find the value of the activation energy, E_a

that would give a doubling of reaction rate between 0 °C and 10 °C, i.e., for $\frac{k_2}{k_1} = 2$

where k_1 and k_2 are the rate constants at absolute temperatures T_1 and T_2.

Then with this value of E_a we shall see what the effect is on $\frac{k_2}{k_1}$ at two different 10 °C ranges.

For the calculation of E_a, take $\frac{k_2}{k_1} = 2$, $T_1 = 273$ K, $T_2 = 283$ K and $R = 8.314$ J K^{-1} mol^{-1}:

Arrhenius equation:

$$\ln\left(\frac{k_2}{k_1}\right) = \left(\frac{E_a}{R}\right)\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

Therefore:

$$\frac{\ln\left(\frac{k_2}{k_1}\right)}{\left(\frac{1}{T_1} - \frac{1}{T_2}\right)} = \frac{E_a}{R} \Leftrightarrow E_a = \frac{\ln\left(\frac{k_2}{k_1}\right)}{\left(\frac{1}{T_1} - \frac{1}{T_2}\right)} \times R$$

Substituting the values given, we have:

$$E_a = \frac{0.693}{\left(\frac{1}{273} - \frac{1}{283}\right)} \times 8.314 = 44500 \text{ J mol}^{-1}$$

= 44.5 kJ mol^{-1}.

It is assumed in this calculation that $\frac{k_2}{k_1}$ does not vary with temperature or the value of the activation energy.

Enthalpies of combustion of alcohols

A linear relationship is predicted between the change of the enthalpy of combustion of monohydric alcohols and the number of carbon atoms. It is predicted that there will be a similar difference from one monohydric alcohol to the next as the homologous series is ascended.

These predictions arise because each methylene group, -CH_2-, is responsible for a fixed increment in the enthalpy of combustion. In addition, each bond makes a characteristic contribution to the enthalpy of the alcohol.

When an alcohol undergoes complete combustion the bonds between the atoms within the alcohol molecule are broken and carbon, hydrogen and oxygen atoms are released. New bonds form between carbon and oxygen atoms to form carbon dioxide and between hydrogen and oxygen atoms to form water (see *Figure 202*). Each alcohol has one more carbon-carbon bond and two more carbon-hydrogen bonds than the previous alcohol. As the alcohol molecules increase in molar mass, more energy is required to break the bonds, but even larger amounts of energy are released as these atoms form carbon dioxide and water. Upon combustion, each alcohol molecule forms one more carbon dioxide molecule and one more water molecule than the previous alcohol.

CH_3OH (l) + $^3/_2O_2$ (g) → CO_2 (g) + $2H_2O$ (l)

C_2H_5OH (l) + $3O_2$ (g) → $2CO_2$ (g) + $3H_2O$ (l)

C_3H_7OH (l) + $^9/_2O_2$ (g) → $3CO_2$ (g) + $4H_2O$ (l)

C_4H_9OH (l) + $6O_2$ (g) → $4CO_2$ (g) + $5H_2O$ (l)

NAME OF ALCOHOL	C-C BONDS BROKEN	C-H BONDS BROKEN	C-O BONDS BROKEN	O-H BONDS BROKEN	O=O BONDS BROKEN	C=O BONDS FORMED	O-H BONDS FORMED
METHANOL	0	3	1	1	1.5	2	4
ETHANOL	1	5	1	1	3	4	6
PROPAN-1-OL	2	7	1	1	4.5	6	8
BUTAN-1-OL	3	9	1	1	6	8	10

Figure 202 Summary of bonds broken and formed during combustion of monohydric alcohols

There is a constant difference between the monohydric alcohols as the homologous series is ascended:

1 extra C—C bond is broken = 1 × 348 = 348 kJ extra energy needed

2 extra C—H bonds are broken = 2 × 412 = 824 kJ extra energy needed

1.5 extra O=O bonds are broken = 1.5 × 496 = 744 kJ extra energy needed

Hence, total extra energy needed = 348 + 824 + 744 = 1916 kJ mol^{-1}

2 extra C=O bonds are formed = 2 × 805 = 1610 kJ extra energy produced

2 extra O—H bonds are formed = 2 × 463 = 926 kJ extra energy produced

So, total extra energy produced = 1610 + 926 = 2536 kJ mol^{-1}

The extra energy released is greater than the extra energy needed and thus, as the homologous series is ascended, the enthalpies of combustion become more exothermic. More importantly, because the change in the structures of the alcohols is fixed, the difference in the enthalpy of combustion from one homologue to the next will also be fixed and will be: ΔH = (1916 – 2536) kJ mol^{-1} = -620 kJ mol^{-1}.

This means that one mole of ethanol will release 620 kJ more energy than one mole of methanol when combusted; one mole of propan-1-ol will release 620 kJ more energy than one mole of ethanol when combusted, and so on. The position of the alcohol functional group (-OH) will have little effect since it is the number and type of bonds that are being broken and made that dictate the size of the enthalpy change of combustion.

Exercise

Carry out a similar exercise with the first four members of the alkanes homologous series. Refer to the IB chemistry data booklet for the relevant data.

Predictions

Predictions are based upon your hypothesis. They are descriptions of what you expect to observe and why.

For example, if you predict first kinetics for a reactant in a particular chemical reaction then you would predict its initial rate of reaction will double if the concentration of the reagent is doubled.

This behaviour can be accounted for by the doubling in the number of collisions involving that reactant in the rate determining step, that is, the elementary step that exerts a dominant effect on the overall rate.

It is important to realise that reaction mechanisms are simply theories, and cannot be proven beyond doubt. Research Chemists are led to accept a theory of the mechanism of a particular reaction because it provides the most satisfactory or easiest approach to understanding the observed kinetic behaviour of that reaction. However, new results may later be obtained which are not consistent with this theory, which must then be rejected or modified.

Consider the replacement reaction between zinc powder and aqueous copper(II) sulfate solution. Since zinc is more reactive than copper (it is higher up in the reactivity or activity series), it is predicted to be able to replace copper from a solution of copper(II) sulfate. (This could also be predicted from a consideration of standard electrode potential data: zinc is a more powerful reducing agent than copper).

If the mass of zinc powder is increased, then the mass of copper replaced should also increase. You must provide a chemical explanation for this qualitative prediction.

$Zn\ (s) + Cu^{2+}\ (aq) \rightarrow Zn^{2+}\ (aq) + Cu\ (s)$

An appropriate ionic equation should be provided which should be explained in words, for example, 'one atom of zinc displaces one atom of copper'. Therefore if the mass of zinc increases and the number of atoms of zinc increases, this will cause the number of copper ions replaced and therefore the mass of copper produced to also increase.

A quantitative prediction and explanation should then be given, for example, if the number of atoms of zinc doubles then the number of atoms of copper replaced will also double (assuming that the copper(II) sulfate solution is present in excess). This means that the mass of zinc used is directly proportional to the mass of copper displaced, but the masses will not be in a 1:1 ratio by mass, since the two metals have different relative atomic masses. Suitable calculations involving the mole concept must be included to support the statement.

2.3 The Investigative Process

2.3.1 Selecting, manipulating and controlling variables

Guiding questions:

- *To what extent has the student devised a methodology that shows awareness of the factors that may influence the collection of data relevant to the Research Question?*

Variables

Variables are factors that can be measured and/or controlled. Independent variables are those that are manipulated, and the result of this manipulation leads to the measurement of the dependent variable. A controlled variable is one that should be held constant so as not to obscure or hide the effects of the independent variable on the dependent variable. The variables need to be explicitly identified by you as the dependent (measured), independent (manipulated) and controlled variables (constants). Relevant variables are those that can reasonably be expected to affect the outcome. For example, consider the Research Question, 'How does changing the acid catalyst concentration affect the rate of the esterification reaction between propan-1-ol and propanoic acid?'

You must clearly state that the independent variable is the concentration of concentrated sulfuric acid (the catalyst and dehydrating agent) and the dependent variable is the concentration of propanoic acid after a fixed time interval. The relevant controlled variables are temperature of the reaction mixture, the initial concentrations in the reaction mixture of propan-1-ol and propanoic acid and any solvent, so that one concentration can be varied independent of the others.

Control of variables refers to the manipulation of the independent variable and your attempt to maintain the controlled variables at a constant value. Your method should include explicit reference to how the control of variables is achieved. If the control of variables is not practically possible, such as atmospheric pressure, some effort should be made to monitor the variable(s).

A standard measurement technique, for example, a redox titration or a flame calorimeter, may be used as part of a wider investigation but it should not be the focus of that investigation. You will be assessed on your individual design of the wider investigation. If a standard measurement technique is used you should reference it.

For example, while planning an investigation to study the factors that influence the rate of oxidation of vitamin C in fresh fruit juices, you may have adapted a method, for example, an acid-base titration or redox titration, for vitamin C determination from a literature source. A standard reference would then be expected as a footnote in your investigation 'write-up'.

A variable is a factor present in an experiment that can be changed and controlled to see what effect it has on the results of the experiment. Each chemical test should change only one variable at a time, in other words, each test should be a fair test. If more than one variable is changed during a test, it will not be possible to conclude which variable was responsible for the change in results.

For example, in the reaction between zinc and dilute aqueous hydrochloric acid the following continuous variables (variables that can be expressed as a decimal number) affect the rate of reaction: temperature of the aqueous hydrochloric acid, concentration of the aqueous hydrochloric acid (assuming the zinc is present in a large excess) and the surface area of the zinc (assuming the acid is present in a large excess). A change in the surface area of the zinc has a much greater effect on the rate than either changing the amount of zinc or acid.

Note that the rate of reaction is not affected by a change in the mass or amount of zinc (in grams or mol) used in the tests. The acid and the metal are also variables and are known as categoric variables (variables that can only be described by words). The initial rate will also be independent of the volume of hydrochloric acid (assuming the zinc is covered), though the way the rate changes with time will be affected.

Consider a simple practice investigation into the replacement reaction between zinc and aqueous copper(II) sulfate. For example, a possible Research Question could be to find the relationship between the mass of zinc and mass of copper produced in the replacement reaction between zinc and copper(II) sulfate.

You need to carefully identify all the variables in the investigation, for example: the mass of zinc powder (independent variable), the mass of copper produced (the dependent variable) and the controlled variables (to make the investigation a fair test): concentration and volume of aqueous copper(II) sulfate solution, temperature, time taken for reaction and the time left to dry the copper powder before weighing.

Consider another simple practice investigation into the effect of particle size on the rate of reaction between calcium carbonate and dilute aqueous acids (in a thermostatted water bath).

A possible Research Question could be to determine the effect of particle size on the rate of reaction between calcium carbonate and dilute hydrochloric acid.

The independent variable is the size of the particles (powder, small grains and large chips); the dependent variable is the time take for the calcium carbonate to react completely (that is the time effervescence occurs); the controlled variables will be temperature, type of acid used, volume of acid and concentration of the acid. It is assumed that the heat released during the reaction will be absorbed by the water bath and will not affect the rate of reaction. It is also assumed that the salt produced when the carbonate reacts with acid has virtually infinite solubility in water.

The identification and control of variables is an important part of IB Chemistry coursework. It may be helpful (where relevant) to have a separate section in your 'write-up' under the heading 'Exploration' that explicitly identifies and classifies the variables inherent in your investigation. The control of variables is the essential difference between scientific experimentation and trial-and-error.

Figure 203 (below) summarises the variables that affect selected various chemical and physical processes or reactions. These processes and reactions would make very suitable practice investigations where the Exploration criterion is assessed.

Chemical/Physical process or reaction	Major variables
Conductivity of an aqueous electrolyte	Strength of electrolyte, nature of electrolyte, temperature and concentration
Hydrolysis of a vegetable oil	Concentration of lipase, concentration of oil, type of oil, presence of detergent (concentration and type), pH, temperature
Solubility of a sparingly soluble ionic compound	Temperature, presence of common ions
Development of oxidative rancidity in an oil	Temperature, light, oxygen concentration, type of oil
Simple electrochemical cell	Nature of electrodes, temperature, immersion area of electrodes, distance between electrodes, concentration of electrolyte
Electroplating in aqueous solution	Current density (current per unit area of the cathode), temperature, presence of other ions and time
Electrolysis of aqueous sodium chloride	Concentration, temperature, distance between the electrodes, immersion depth of electrodes
Hydrolysis of halogenoalkanes	Nature of halogen atom, nature of carbon backbone, nature of solvent, temperature and pH
Thiosulfate ions and hydrogen ions reaction rate in aqueous solution	Concentrations of reactants, temperature, presence of a catalyst e.g. iron(III) ions
Formation of an ester from an alcohol and a carboxylic acid (equilibrium constant)	Use of excess reagent, removal of ester (via distillation), length of reflux time

Figure 203 Variables affecting common chemical processes or reactions

Exercise

Magnesium blocks are used to provide protect to iron objects, such as ships and piers.

- Design an experiment to investigate the effect of corrosion by sea water on magnesium.
- Identify the independent, dependent and controlled variables.

2.3.2 Establishing the rationale for the method

Guiding questions:

- ***To what extent does the methodology allow for the collection of sufficient relevant data that could enable a reasoned conclusion to be drawn?***
- ***To what extent has the student shown how their method has been developed and modified?***
- ***When appropriate, to what extent does the investigation indicate an awareness of safety, environmental, and ethical considerations?***
- ***To what extent does the student engage with the investigation and make it their own?***

Planning a scientific investigation is one of the most demanding and difficult skills to learn. In order for training in planning skills to be effective you must have confidence in your practical abilities. It is not sufficient that you have simply learnt to follow instructions; you must be able to apply the experience you have got from earlier exercises in order to see the consequences of a given choice on the outcome of your plan. It is therefore vital that you understand the rational for using particular approaches, pieces of equipment, recording and analysing techniques, rather than simply performing a given exercise in a particular prescribed way.

An appreciation of precision and reliability is essential when choices of measuring equipment or apparatus are made, and when experimental procedures are suggested. An understanding of random errors and possible systematic, associated with individual pieces of apparatus is fundamental to the successful choice of apparatus for a given task. A similar argument applies to the identification of variables that need to be controlled, and the proposing of suitable measures to control them.

The advantages and limitations of one type of measuring device, control measure or practical approach compared to other possibilities must be understood if the appropriate equipment, approach and quantities are to be used. The proposed experimental procedure should be workable. It should, given that the apparatus is assembled appropriately, allow data to be collected without great difficulty.

There should be a description, including labelled diagrams in cross section, of how the experiment should be performed and how the key variables are to be controlled. However, drawings perhaps should be perhaps be limited to complex set-ups, non-standard equipment or standard equipment being in an unusual manner.

Equipment or apparatus, of a level of precision appropriate for the measurements to be made, and quantities (and concentrations) of chemicals (IUPAC names and formulas) to be used should be specified.

The use of control experiments should be considered, if appropriate, especially if enzymes are present. Also, details of how the raw data are to be recorded, manipulated, analysed and evaluated should be given. Your method should not be a 'recipe' or simple list. It should justify the techniques and apparatus selected. It is suggested that it is in two sections: the planning and development of the method and the method actually used.

You may build your own apparatus for use in your Individual Investigation, for example a simple polarimeter (to study optical activity in sugars) or an Evans balance (to measure paramagnetism in transition metals salts).

You may also be using a standard method such as dual indicator approach together with a data-logger to record pH. You may also be using column chromatography with a vacuum pump to carry out 'flash chromatography'. It is very important to document and justify any modifications to standard methods. For example, you may have had to dilute a solution to get better titration results. There may be a need for controls. For example you may have made up a solution of known concentration to check the accuracy of one or more techniques.

Method

Your method should clearly allow another IB Chemistry student to replicate your Individual Investigation and results (within experimental error). *Figure 204* shows two lists of the same apparatus and materials used for a simple practice investigation that is assessed against the Exploration criterion.

Student A	Student B
Apparatus	**Apparatus**
Beakers	2 × 250 cm^3 glass beakers
Balance	Electronic balance (±0.0001 g)
Volumetric flask	50.00 cm^3 volumetric flask (TC) (±0.05 cm^3)
Burette	50.0 cm^3 burette (TD) (±0.1 cm^3)
Pipette	50.0 cm^3 pipette (TD) (± 0.05 cm^3)
Thermometer	Mercury thermometer (-10 to + 110 °C, ± 0.2 °C)
Conical flasks	3 × 100 cm^3 glass conical flasks
Clock	Manually operated electronic stop watch (± 1 s)
Spatula	Nickel spatula
Data logger	pH data logger sensor (manufacturer: Vernier Logger Pro 3.1: ± 0.02 pH units).
Chemicals	**Chemicals**
Methanoic acid	2.00 mol dm^{-3} methanoic acid, HCOOH(aq)
Propanoic acid	2.00 mol dm^{-3} propanoic acid, $C_3H_7COOH(aq)$
Sodium carbonate	10.00 g of sodium carbonate-ten-water, $Na_2CO_3.10H_2O(s)$
Potassium hydroxide	0.0915 mol dm^{-3} potassium hydroxide, KOH(aq)

Figure 204 Comparing equipment lists

Student A's list is imprecise and hence the method is not reproducible. Any deviations from the original method given or suggested by you should be documented and justified.

Most importantly you must carefully make sure that you have described a fair test. For example consider again the replacement reaction between zinc powder and aqueous copper(II) sulfate solution.

Here is what a student might think or write during a simple practice investigation into metal ion replacement that is going to be assessed against the Exploration criterion.

'*Every time I change the mass of zinc powder I will use the same volume and concentration of aqueous copper (II) sulfate (present in excess – I will provide a calculation to prove this). I will perform the experiment at the same temperature in the same clean, dry glass apparatus and leave the mixture to react for the same period of time in the same air-conditioned laboratory. I will leave the copper to dry for the same length of time in a thermostatted oven (at the same temperature) before weighing (on the same electronic balance)*'.

Finally your method must include a description of sufficient raw data that you intend to collect. This means that you need to suggest how many times you should change variables and the values that you will use.

For example, consider changing the mass of zinc powder added during an investigation of the replacement reaction between zinc powder and aqueous copper(II) sulfate solution.

'*I will use approximately 0.5 g of zinc powder the first time and record the precise mass and then the following approximate values 1.0 g, 1.5 g, 2.0 g, 2.5 g and 3.0 g and record the precise masses so that six tests are performed*'.

Always make sure that you suggest at least five different and equally spaced values (unless it is not appropriate).

What will you measure?

For example, 'I will be measuring the mass of the dry copper powder produced after each experiment'. What will I control?'

For example, the volume of aqueous copper(II) sulfate solution used will be 50.0 cm^3 (heated to a temperature of 50.0 degrees Celsius) and its concentration will be 1.50 mol dm^{-3} to ensure that it is present in excess (see appendix for calculation). I will leave each hot reaction mixture for 10 minutes to react (in an open 100 cm^3 glass beaker). I will stir for two minutes after the reaction begins. I will also allow each sample of copper powder to dry for twenty four hours in an oven at 80 °C for 4 hours before weighing'.

How will you ensure accuracy?

'Each experiment will be repeated three times and then averaged to obtain accurate and reliable results for each mass of zinc used'.

Organic chemistry preparations

A reporting style, with quantities in brackets after each chemical reactant or solvent, is often favoured for an organic investigation. For example:

'Sodium metal (2.65 g; 0.12 mol) was added, a little at a time with caution, to ethanol (75.00 cm^3) in a round-bottomed flask fitted with a reflux condenser.

The solution became warm and a gas (assumed to be hydrogen) was evolved as the sodium reacted. After 15 minutes…'

Where applicable describe the chemical reaction by writing a balanced or stoichiometric equation at the beginning (*Figure 205*). Displayed structural formulas are normally more helpful than molecular formulas. Include the relative molecular masses or molar masses of the reactants and products, the mass of the limiting reagent and hence the theoretical yield.

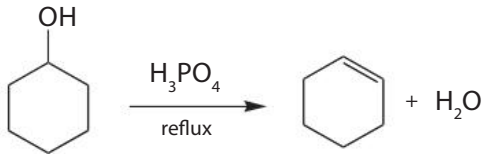

Figure 205 Skeletal formula showing the dehydration of cyclohexanol to form cyclohexene

It may also be helpful to explain and justify the use of particular organic practical techniques. For example, you may reflux ethanol with acidified potassium dichromate(VI) to form ethanoic acid. The refluxing is to ensure that any ethanal (an intermediate oxidation product) is cooled, condensed (by the cold glass wall of the reflux condenser and returned to the hot reaction mixture for further oxidation to ethanoic acid.

When you have prepared and purified an organic product, give the experimental yield in grams and then as a percentage of the theoretical yield.

Measure and record physical data required such as the melting point (range) if the product is a solid or its boiling point (range) if a liquid, together, for the purposes of comparison, with values from the chemical literature–most likely a data booklet or a text book appendix.

For example:

… produced X as a colourless liquid (6.6 g; 30%), boiling point 68-72 °C at one atmosphere pressure;

(literature boiling point 70 °C at one atmosphere pressure. (*Dictionary of Organic Compounds* (3rd edition), Singapore University Press, 1997.)

On-line resources for practical work

The Royal Society of Chemistry has information on a range of standard chemical techniques including associated health and safety guidance (*Figure 206*).

The URL is <*http://www.nuffieldfoundation.org/practical-chemistry/standard-techniques*> used with permission (see below).

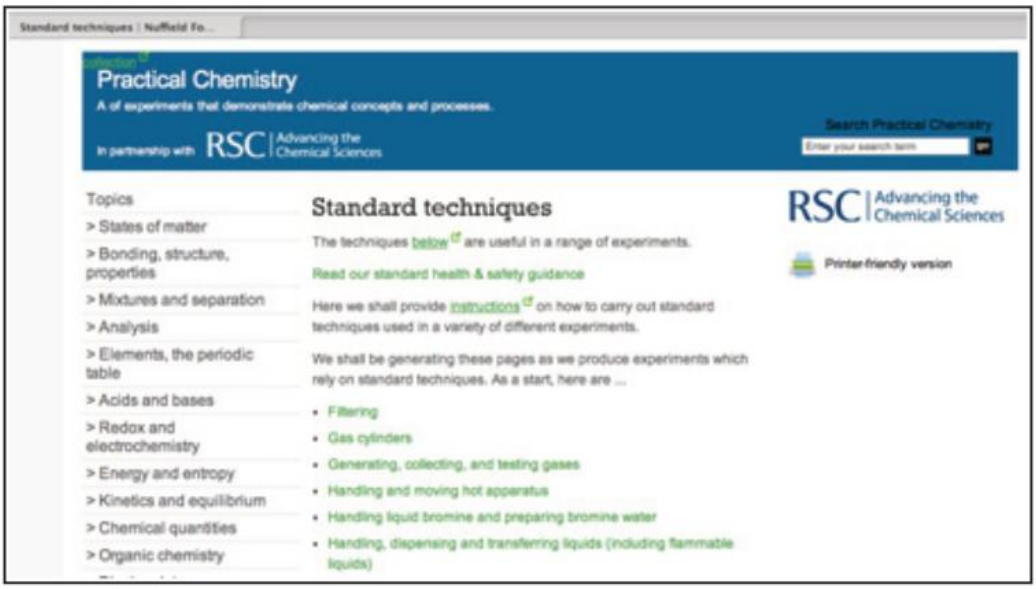

Figure 206 Website for The Royal Society of Chemistry

The Royal Society of Chemistry has another web site that shows various experimental techniques including organic techniques, such as refluxing and distillation.

The URL is <*http://www.rsc.org/Education/Teachers/Resources/practical/*> (*see Figure 207*)

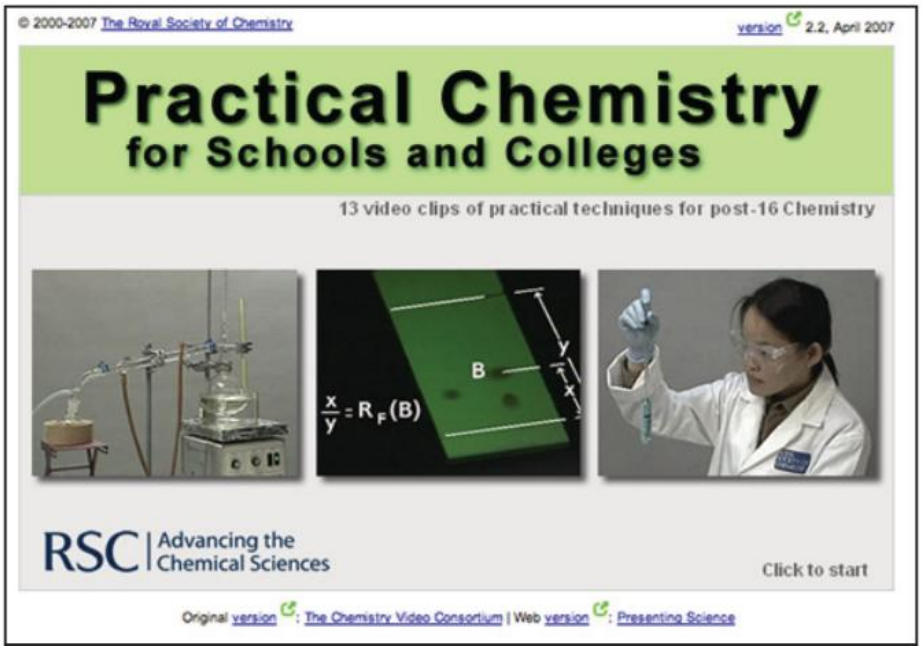

Figure 207 Information about Practical techniques

Drawing Chemical Apparatus for a Design Investigation

General guidelines for drawing good diagrams of Chemical apparatus for the planned method of a practice investigation being assessed against the Exploration criterion.

- Draw diagrams in cross section, not as three-dimensional pictures.
- Start at the top of your lab book page and work downwards, so that you are less likely to run out of space.
- Make drawings sufficiently large so the detail can be seen.
- Do not draw Bunsen burners, the bench, gas taps or clamps.
- A water or an oil bath should be shown if used.
- Label important points on the diagram or unusual items.
- If you name the glassware, then use the correct names.

Simple Distillation

Note the following points:

- The bulb of the thermometer is located opposite the entrance to the condenser since you want to record the temperature of the vapour.
- The delivery bend is vented so that when the apparatus is heated the glass joints are not pushed apart by the expanding gas.
- Never draw closed apparatus.

Note the internal structure of the Liebig condenser: the water jacket is separate and sealed from the tube that runs down the middle.

Heating Under Reflux

Note the following points:

- The water enters at the bottom of the Liebig condenser and leaves from the top.
- There must not be a stopper inserted into the top of the condenser – the apparatus must not be sealed.
- No thermometer should be placed into the top of the condenser

A description and diagrams of refluxing and distillation (simple and fractional) may be found elsewhere. *Figure 208* is a cross sectional diagram showing the standard laboratory preparation of hydrogen gas. It is provided as an example of a well drawn and labelled diagram.

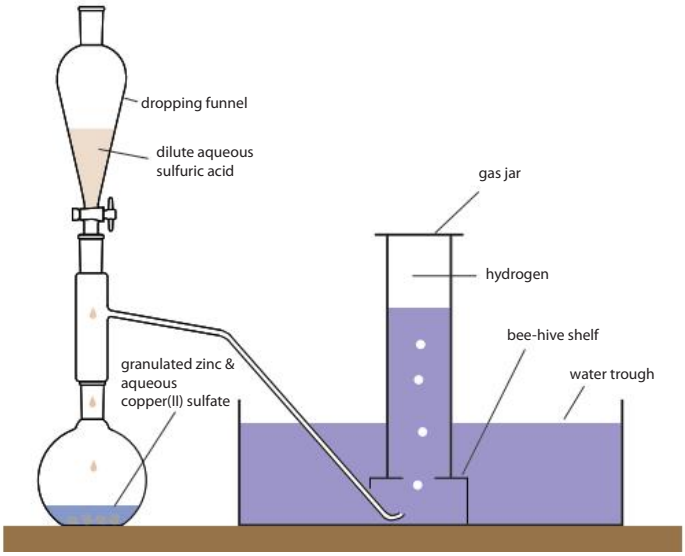

Figure 208 Collection of hydrogen gas

Experimental procedures for an Exploration Investigation

A number of issues have to be considered in a successful experimental design for an IB Chemistry Individual Investigation. Listed below are some questions that should be asked during the design of any experimental procedure involving a chemical reaction. You should get into the habit of asking appropriately critical questions of every practical procedure that you have experienced during your IB Chemistry practical programme.

- In quantitative experiments, have the quantities (masses and/or volumes) been calculated correctly and are they are of a reasonable magnitude?
- In a preparation, is the scale on which it is planned appropriate for the aim?

  The use of small quantities during organic or medicinal chemistry experiments can often result in little or no yield, simply due to mechanical losses. However, the use of large reacting quantities may raise waste and safety considerations.

- Have the quantities of each reagent been calculated correctly?

  Thus, if a particular reagent has to be present in excess, for example, during a kinetics or replacement investigation, the calculation will need to be checked.

- Are the concentrations of the solution used in an investigation, for example a titration, reasonable?

  Use of very concentrated solutions may give rise to inaccuracy, since one drop of the reagent solution contains a relatively large amount of dissolved solute in terms of the likely error or uncertainty in the measurement of the solution volume.

Conversely, the use of very dilute solutions may give rise to relatively large titre volumes, which means the burette has to be refilled. It reduces the percentage error, but it increases costs and also gives less flexibility for a titre being higher than expected.

If a titration is planned then you should aim to use concentrations of approximately 0.1 mol dm^{-3} and have an end point between 15 and 40 cm^3. This will ensure that the last drop at the end point contains only a relatively small amount of reagent.

It is usually best to use the same concentration for the two reacting solutions. However, there are exceptions to this:

- For the reaction between aqueous sulfuric acid (dibasic) with aqueous sodium hydroxide it is best to use 0.05 mol dm^{-3} sulfuric acid with 0.1 mol dm^{-3} sodium hydroxide in order to keep the volumes identical.

  H_2SO_4 (aq) + 2NaOH (aq) → Na_2SO_4 (aq) + $2H_2O$ (l)

- For redox titrations, the 'electron concentration' should be approximately 0.10 mol dm^{-3}. Potassium manganate(VII) is therefore normally used at a concentration of 0.02 mol dm^{-3}.

  MnO_4^- (aq) + $8H^+$ (aq) + $5e^-$ → Mn^{2+} (aq) + $4H_2O$ (l)

  In experiments involving the measurement of heat changes, the situation is different since you need to produce a conveniently measurable temperature change. In order to produce a significant temperature rise then more concentrated solutions are required, of the order of 1 or 2 mol dm^{-3}.

  A relatively large volume of solution is preferable since its surface area to volume ratio for heat loss is minimised. It is also easy to stir without the risk of spillage.

- If limits have been set on the amount of material or substance to be weighed out, have these limits been adhered to?

It is necessary to know the number of times the test is likely to be replicated. For example, if a standard solution needs to be prepared for a titration, then 250 cm^3 is more than sufficient and will allow up to nine sets of results using 25 cm^3 aliquots.

Safety

All practical work should be carried out in accordance with the health and safety legislation of the country in which it is done. You should not attempt any activities that conflict with this legislation and all your planned investigations must be approved by your chemistry teacher. Some safety information is provided in the front of the book.

Hands-on practical work can be carried out safely in schools but to ensure that it is safe, you must identify the hazards and reduce any associated risks to insignificant levels by adopting suitable control measures.

Risk assessment involves answering two basic questions:

How likely is it that something will go wrong?

For example, if you are pushing a delivery tube through a tight bung it is possible that the tubing will break and cut you.

How serious would it be if it did go wrong?

For example, the consequences of a spark from an experiment landing in an open bottle of magnesium powder are likely to be serious, and include spraying burning magnesium all over the laboratory, perhaps burning many students and setting the chemical laboratory ceiling on fire.

Once you have the answers to these questions, it is possible to plan your Individual Investigation to minimise the risk of an accident occurring and, if it does, to minimise its possible severity. In the second example, this could include bringing only the amount of magnesium powder required for the activity into the laboratory and making sure other students are aware of the magnesium powder.

Eye protection is the main control measure for preventing injury and glasses or goggles should be worn at all times in the laboratory. If you expect a problem, a range of control measures may be adopted, the following being the most common.

Use:

- a less hazardous (substitute) chemical.
- as small a quantity as possible.
- as low a concentration as possible.
- a fume cupboard and safety screens.

Shown below are the stages in carrying out a Risk Assessment for an IB Chemistry Investigation

1. Write down the chemicals and procedures you will be using (chemicals used or made, quantities, concentrations (if solutions), techniques and non-chemical hazards).
2. Use reference sources to identify any hazardous chemicals you are planning to use or make. Warning symbols will be printed on reagent bottles and in supplier's catalogues.
3. Record the type of hazards involved and the way you might be exposed to the hazard. There are standard reference sources with this information, such as the 'Hazcards' published in the United Kingdom by CLEAPSS. In North America MSDS (material safety data sheets) sheets should be read (*Figure 209*). Ensure you consult reliable sources such as chemical manufacturers, chemical societies and safety bodies.

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Sodium hydroxide	1310-73-2	100

Toxicological Data on Ingredients: Sodium hydroxide LD50: Not available. LC50: Not available.

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (corrosive, irritant, permeator), of eye contact (irritant, corrosive), of ingestion, of inhalation. The amount of tissue damage depends on length of contact. Eye contact can result in corneal damage or blindness. Skin contact can produce inflammation and blistering. Inhalation of dust will produce irritation to gastro-intestinal or respiratory tract, characterized by burning, sneezing and coughing. Severe over-exposure can produce lung damage, choking, unconsciousness or death. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to mucous membranes, upper respiratory tract, skin, eyes. Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure of the eyes to a low level of dust can produce eye irritation. Repeated skin exposure can produce local skin destruction, or dermatitis. Repeated inhalation of dust can produce varying degree of respiratory irritation or lung damage.

Figure 209 MSDS card for sodium hydroxide

- Decide what protective or control measures to take so that you can carry out your practical work healthily and in safety.
- Find out how to dispose safely of any hazardous residues from your practical work and record this in your report with your reference.
- Check your plans with your Chemistry Teacher before starting any practical work.

An example of a Chemistry Investigation Risk Assessment form is shown in the Figure below.

<table>
<tr><td colspan="4">TITLE OF THE IB CHEMISTRY INDIVIDUAL INVESTIGATION</td></tr>
<tr><td colspan="4">Outline of the procedures</td></tr>
<tr><td>Hazardous substances being used or made</td><td>Nature of the hazards (e.g. highly flammable, toxic)</td><td>Quantities and concentrations being used or made</td><td>Safety measures (precautions)</td></tr>
<tr><td></td><td></td><td></td><td></td></tr>
<tr><td colspan="3">Any non-chemical hazards and precautions to be taken</td><td>Signed (student)
.....
Signed (Teacher)
.....</td></tr>
<tr><td colspan="3">Disposal of residues</td><td>Date:
.....</td></tr>
</table>

Handling Chemicals

You should regard all the chemicals you handle in the chemical laboratory to be hazardous. The most commonly used 'dangerous' chemicals are acids (>2 mol dm^{-3}), halogens in solution and alkalis (>2 mol dm^{-3}). All of these are corrosive and will damage skin and eyes. If you have an accident or spill acid, halogen or alkali then wash the chemical off with lots of running water and immediately report the accident to your Chemistry Teacher.

Another group of 'dangerous chemicals' are oxidising agents, such as potassium dichromate(VI), $K_2Cr_2O_7$, and potassium manganate(VII), $KMnO_4$. These substances, when in solid form, may produce large amounts of heat as they react with other substances. They can create a fire risk. Your Chemistry Teacher will warn if there is any potential hazard with chemicals made available for your Individual Investigation or for chemicals that you have requested for a planned investigation.

You must make careful note of any safety instructions your Chemistry Teacher gives you. Look for the safety symbols shown in *Figure 210* which indicate you need to wear gloves and goggles. You must also read any practical instructions, noting any warnings given. You must also look at the labels on the reagent bottles. There are international symbols for chemical hazards and these are shown in the front of this publication.

Make sure you get information about chemicals before you start to use them. If you are using solutions it is much easier to use the correct solution if you already have a mental image of Benedict's solution as the 'blue solution', iodine solution as the 'brown solution'. Where possible use colours to distinguish between chemicals. If the chemicals are colourless or the same colour then make sure you carefully label or mark them carefully.

Figure 210 Some chemical hazard symbols

Sample Risk Assessment

A detailed method needs to be submitted to your IB Chemistry teacher before you can begin your Individual Investigation.

List of reactants and products

Chromium(III) chloride-6-water (solid)	Irritant; harmful by ingestion
Potassium hydroxide (solid)	Corrosive
Chromium(III) hydroxide	Minimal hazards
20 volume hydrogen peroxide solution	Irritant
Potassium chromate(VI) (solid)	Toxic
Glacial ethanoic acid	Corrosive, flammable
Potassium dichromate(VI) (solid)	Toxic (by inhalation)

Risk Assessment

Safety glasses must be worn at all times as potassium hydroxide is corrosive to eyes. Potassium hydroxide and glacial ethanoic acid are corrosive and hence disposable gloves and a buttoned up lab coat should be worn at all times. Inhalation of glacial ethanoic acid may cause lung and tooth damage. Any spillages should be reported immediately to your IB Chemistry Teacher and extensive dilution with water performed. Potassium chromate(VI) and potassium dichromate(VI) are toxic, and chromium(III) chloride and 20 volume hydrogen peroxide are irritants. Skin contact should be avoided. As hydrogen peroxide can be react explosively with glacial ethanoic acid, the school technician should be instructed to dilute and destroy any excess by boiling to decomposition. Potassium dichromate(VI) should be converted to chromium(III) ions by reaction with sodium metabisulfite, $Na_2S_2O_5$.

2.3.3 Establishing the rationale for the data processing

Your plan should include data tables that can be used to record relevant quantitative data. Your plan should also indicate what qualitative date should be recorded, for example, colour changes.

Your plan should also clearly outline how the raw data will be processed. For example, mass differences may be calculated, times (s) may be converted to 'rates' (s^{-1}) and pH values or rate constants may be transformed using a logarithmic function. These involve the conversion of dependent variables into processed variables.

The chemical and mathematical rationale behind the data processing must be clearly outlined in detail in your plan or report for the Individual Investigation.

It is likely that one or more graphs displaying processed data will be generated during your Individual Investigation. The graphs that will be drawn should be outlined, perhaps including sketches with blank axes.

For example if you are planning to generate an Arrhenius plot (of ln *k* versus reciprocal of absolute temperature) the mathematical transformation of the rate constants and times must be described, explained and justified, both chemically and mathematically.

You may be carrying out investigation that involves an acid-base titration where pH is followed by a pH meter. When a weak acid is titrated with a strong base then at the half-neutralisation point pK_a = pH (the pH when half the volume of base required to exactly neutralise the acid has been added to the acid). This needs to be justified mathematically and chemically and any assumptions from acid-base theory outlined.

Any statistics, including simple averaging, must be outlined and justified.

Sample Exploration hypotheses

Below is an example of a series of chemical hypotheses based on a series of related acid-base equilibria. It may make an excellent series of practice investigations for assessing the Exploration criterion.

A variety of Research Questions may be generated from this system. For example, to find the relationship between pH and partial pressure of carbon dioxide above distilled water in a sealed container.

Background information

Carbonated drinks contain carbon dioxide dissolved under pressure. When carbon dioxide dissolves in and reacts with water, several chemical equilibria are established.

Carbon dioxide molecules in the gas phase in the space above the surface of the drink, known as the head space, are in equilibrium with hydrated molecules in the aqueous phase:

$CO_2(g) \rightleftharpoons CO_2(aq)$ $\quad \Delta H^{\ominus}$ is negative

A proportion of the carbon dioxide also reacts with the water to form carbonic acid:

$CO_2(aq) + H_2O(l) \rightleftharpoons H_2CO_3(aq)$

Carbonic acid is a weak acid and dissociates to give hydrogencarbonate and carbonate ions:

$H_2CO_3(aq) \rightleftharpoons HCO_3^-(aq) + H^+(aq)$

$HCO_3^-(aq) \rightleftharpoons CO_3^{2-}(aq) + H^+(aq)$

Carbonated drinks are manufactured by dissolving carbon dioxide gas under pressure in cold water.

Henry's law is approximately obeyed, namely, that doubling the pressure of carbon dioxide will double the amount of gas dissolved in the water.

(This law is only, however, obeyed exactly by an ideal gas that does not chemically react with water).

The loss of carbon dioxide involves a reversal of the equilibria described above:

$CO_3^{2-}(aq) + H^+(aq) \rightleftharpoons HCO_3^-(aq)$

$HCO_3^-(aq) + H^+(aq) \rightleftharpoons H_2CO_3(aq)$

$H_2CO_3(aq) \rightleftharpoons H_2O(l) + CO_2(aq)$

$CO_2(aq) \rightleftharpoons CO_2(g)$

Soda water is acidic due to the presence of hydrogen ions, $H^+(aq)$. The pH of the solution is related to the concentration of hydrogen ions, $H^+(aq)$, present and hence to the concentration of dissolved carbon dioxide, $CO_2(aq)$.

Hypotheses

Effect of temperature on the equilibrium of the system

If a carbonated drink is chilled and its temperature is decreased, then the forward reaction for equilibrium 1 is favoured resulting in more carbon dioxide dissolving in the water and a smaller rate of carbon dioxide bubble production and consequently a decrease in pH.

The forward reaction is favoured due to the system obeying Le Chatelier's Principle, namely, that any change imposed on the system will cause the system to respond by opposing the change. Le Chatelier's Principle is a consequence of a reaction minimising its Gibbs free energy change, ΔG.

If the temperature of the system is lowered then the system responds by increasing the temperature and thus favours the forward reaction of equilibrium 1 which is exothermic, namely, that heat is released into the surroundings. When the temperature is raised the rates of both the forward and reverse reactions are increased, but the rate of the forward reaction is increased by a higher factor.

If a carbonated drink is warmed and its temperature is increased, then the backward reaction for equilibrium 1 is favoured which is endothermic, namely, that heat is absorbed from the surroundings. This results in less carbon dioxide dissolving in the water and greater bubble production and consequently an increase in pH. When the temperature is lowered the rates of both the forward and reverse reactions are increased, but the rate of the backward reaction is increased by a higher factor.

Effect of adding sodium hydrogen carbonate

If a solution of sodium hydrogencarbonate is added to a carbonated drink then there will be an increase in the concentration of hydrogen carbonate ions. Le Chatelier's Principle predicts that equilibrium 3 will shift from right to left to remove it, favouring the backward reaction, which results in equilibrium 2 and then equilibrium 1 also shifting from right to left, resulting in increased formation of carbon dioxide and consequently decrease in pH.

If solid sodium hydrogencarbonate is added to the carbonated drink the chemical effect described above will take place, but the rate at which bubbles are produced is increased due to the introduction of nuclei, that is, sites for the formation of gas bubbles on the solid surface.

Effect of adding hydrochloric acid

Hydrochloric acid will supply hydrogen ions that will shift equilibria three, four and then two and one from right to left resulting in an increased rate of production of carbon dioxide bubbles.

Effect of stirring

When dissolved carbon dioxide escapes from solution and enters the gas phase, this can only occur at the interface between the solution and the atmosphere, that is, at the surface of the solution. Stirring may increase the diffusion of molecules towards the surface and vigorous stirring may also increase the surface area of the interface between the surface of the liquid and the atmosphere by creating bubbles of gas in the liquid. Hence, stirring may increase the rate at which carbon dioxide is lost but on its own would not affect the position of the equilibrium.

Sample Exploration Plan

Below is an incomplete outline plan describing how to address the Exploration criterion when designing a simple kinetics investigation. This practical is probably only suitable as a practice for the Individual Investigation. The author's comments are in italics.

Aim

Investigating the reaction between magnesium ribbon and hydrochloric acid.

Research Question

The aim is to identify the relationship between the concentration of hydrochloric acid and the initial rate of reaction (at constant temperature) as measured by the reciprocal of the time taken for the reaction to go to completion

(Many other variables could be investigated, for example, temperature of the hydrochloric acid, solvent used for the acid, stirring and the surface area of magnesium, metal used, acid used).

Introduction and background

It is assumed that the reaction between magnesium and dilute aqueous hydrochloric acid can be described by the following ionic equation:

$Mg(s) + 2H^+(aq) \rightarrow Mg^{2+}(aq) + H_2(g)$

It is assumed that magnesium atoms do not directly react with the spectator chloride anions. The reaction is a redox reaction with the magnesium changing its oxidation number from 0 to +2 and the hydrogen from + 1 to 0.

It is also assumed that the reaction is sufficiently dilute to ensure that the redox properties of hydrochloric acid are not observed.

It is also assumed that the magnesium is pure and no impurities are present causing release of gas.

Hypothesis

It is predicted that as the concentration of hydrochloric acid is increased the time taken for the reaction to go to completion will decrease. This means that the 'rate' (reciprocal of time) will increase. This can be explained by the increase in collision rate between hydrogen ions and magnesium atoms on the surface of the magnesium. A higher concentration of acid means a higher number of hydrogen ions per unit volume and hence a corresponding increase in the collision rate and hence reaction rate.

(Some simple diagrams illustrating collision theory may be a useful inclusion).

Risk Assessment

Safety glasses and disposable gloves are to be worn at all times. No naked flames will be allowed due to the release of hydrogen. Residual hydrochloric acid will be neutralised with sodium hydrogen carbonate before being flushed down the sink with copious amounts of water. Inhalation of acid spray is to be avoided by maximising the distance from the reacting chemicals. The laboratory must be well ventilated.

Classification of variables

Dependent variable:	Time for reaction to go to completion
Processed variable:	'Rate' (reciprocal of time)
Independent variable:	Concentration of hydrochloric acid
Controlled variables:	Mass and purity of magnesium
	Surface area of magnesium
	Temperature of hydrochloric acid
	Stirring (none)

It is important to control the temperature of the hydrochloric acid and the surface area of magnesium since both affect the rate of reaction. The reaction will be carried out in an air-conditioned laboratory.

(*Stirring can be controlled and quantified by means of a magnetic stirrer; a thermostatted water bath is required for proper control of temperature*).

Materials and apparatus

Magnesium ribbon (99% purity)

(Approximate dimensions: width 3mm, length 22 mm and thickness 0.25mm)

Fine sand paper

Metal rule (±1mm)

2.00 mol dm^{-3} aqueous hydrochloric acid

25 cm^3 pipette 0.06 cm^3 (Class B)

50 cm^3 burette ± 0.1 cm^3 (Class B)

250 cm^3 glass conical flask

Electronic stopwatch (±0.005 s)

Discussion about possible methods and methodologies

A simple and easily reproducible method is to use a fixed length of cleaned magnesium ribbon and time how long it takes for all the metal to react with the acid and form soluble magnesium chloride. The reciprocal of time can be taken as a measure of the rate. This is essentially a variant of the initial rate method.

Note that for this method to be valid, a large excess of acid must be used. Provided that a large excess of hydrochloric acid is used, by the time the magnesium strip has reacted the concentration of hydrochloric acid is still virtually the same as it was at the start, so the rate of reaction throughout the dissolving process only decreases slowly. Therefore, since rate is inversely proportional to time, a measure of the rate can be obtained from the reciprocal of time. It is assumed that the magnesium ribbon will have constant dimensions.

To determine how much of the chemicals I need for the apparatus I plan to use, I need to refer to the stoichiometric equation for the reaction: $Mg\ (s) + 2HCl\ (aq) \rightarrow MgCl_2\ (aq) + H_2\ (g)$

Hence one mole of magnesium reacts with two moles of hydrochloric acid to give one mole of hydrogen and one mole of magnesium chloride.

"To determine the amount of hydrochloric acid I need to know its volume and concentration. To estimate the length of magnesium ribbon I will need to weigh it (after cleaning it thoroughly) on an electronic balance. I will divide the mass by the molar mass of magnesium to obtain the amount in moles. I will then compare the amounts (in mol) of hydrochloric acid and of magnesium. I plan to use ten times as many moles of the acid relative to the magnesium to ensure that the acid is present in excess and the magnesium is the limiting reagent."

(*A clearly explained calculation of the amount (moles) of magnesium from the determined dimensions of the strip must be given.*)

An alternative method is to collect and measure the volume of hydrogen produced over measured time intervals. This would allow me to plot the volume of product formed against time to and to determine the rate at selected times by finding the gradient of the graph at these times.

This could be done by collecting the gas in a sealed gas syringe in the apparatus shown below in *Figure 212* However, this approach may not give such reliable results as the method chosen since it may be difficult to make the apparatus air tight, the gas syringe may stick.

(It is perfectly acceptable and indeed you are encouraged to explore alternative methods and justify why they were not employed).

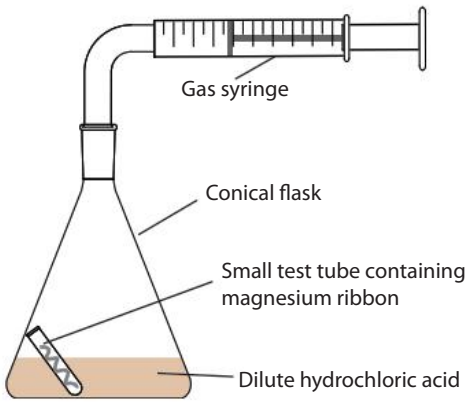

Figure 212 Using a syringe to collect gas

A clear and reproducible method must also be given. Each experiment at one concentration of hydrochloric acid must be repeated before the acid concentration (independent variable) is changed.

(Blank results tables also need to be given and an outline of the data processing, which in this investigation would include averaging and calculating reciprocals. A sketch of the expected graphical relationship between the independent and dependent variable may also be helpful.)

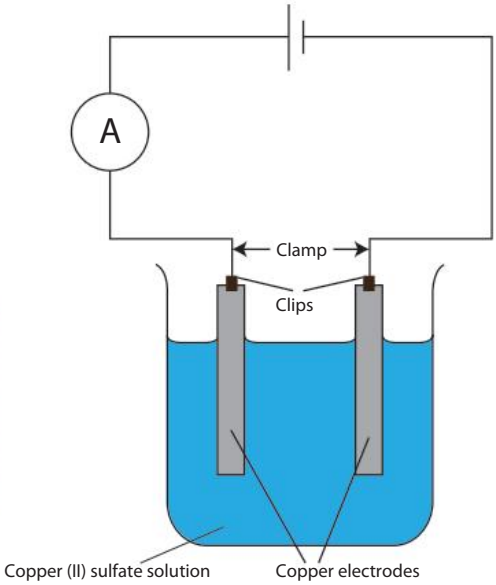

Figure 213 Electroplating apparatus

Exercise 1

Refer to the setup in *Figure 213*. The electrodes are clean copper sheets. Try to generate a focused Research Question and identify and classify relevant variables.

Exercise 2

Suppose you are carrying out a simple investigation to verify Boyle's law: the relationship between the pressure and volume of a gas at constant temperature. Generate a table classifying the variables and stating a method for their measurement/control and a reason for the control of the controlled variables.

2.4 Use Of Apparatus And Instruments

It is important that you are able to effectively and safely handle chemicals and laboratory equipment, set up chemical apparatus properly, and safely and competently perform out a range of successful practical procedures. Your risk assessment and safety considerations during these your Individual Investigation and practice investigations will be assessed. An ability to be able to adapt to changing circumstances during an investigation is also critical.

You will also be assessed on your attention to environmental issues involved in your investigation. This could be demonstrated by wastage of materials or resources, for example, distilled water, and improper disposal of chemicals and waste during your practical. Safety issues should always be clearly addressed and chemical spillages should always be dealt with in the appropriate manner. Chemical apparatus and chemicals must also be stored away safely and effectively.

The correct use of common laboratory apparatus and the development of good techniques will allow you to score highly in the Exploration and the Analysis criteria. They will also help reduce random errors and prevent systematic errors.

Volumetric Glassware

Pipette

Always rinse the pipette with a small quantity of the solution to be measured before beginning the titration. Discard this rinse solution. Check that the tip of the pipette is not damaged before use. Ensure the tip of the pipette is placed well below the surface of the solution before using a pipette filler to draw the solution above the scratch mark. Wipe the outside of the pipette after filling it with solution.

Allow the excess solution to run out into a beaker until the meniscus is on the scratch mark. Check that no air bubbles are present, especially at the tip. Remove the pipette filler and allow the solution to drain naturally for thirty seconds before touching the tip to the inside of the flask for about three seconds. This allows the correct retention of the last drop of the solution by the pipette: do not attempt to remove it by blowing. Check that the pipette drains cleanly without leaving drops clinging to the side. If it does not, it will need a thorough cleaning with detergent.

Burette

Rinse this with the solution you are going to put in it. Make sure you rinse through the tap and jet. Discard the rinse solution. Fill the burette to above the 0.00 cm^3 mark. Run out excess solution into a beaker to fill the tap and jet, check no air is trapped in the jet. Loss of bubbles will add to the measured volume even though no corresponding solution is delivered to the flask. There is no need to adjust the volume of solution to exactly 0.00 cm^3 (but it may reduce the risk of arithmetical errors). Remember to remove the filter funnel used to help fill the burette.

Aqueous solutions of alkalis are generally not placed into burettes since they gradually absorb carbon dioxide from the atmosphere forming deposits of solid carbonates. The presence of alkali in a burette may therefore lead to the jet being blocked and can also lead to deposits of solid carbonates in the socket of the burette tap. This makes the tap difficult to clean and, additionally, the alkali could slightly dissolve the glass causing the ground glass of the stopcock and socket to fuse together.

Readings should always be taken with the eye level with the bottom of the meniscus. It also helps to use a 'burette reader' (see *Figure 214*): a piece of card behind the burette, the upper half being white and the lower half black (which is positioned just below the meniscus). A magnifying glass can also be used.

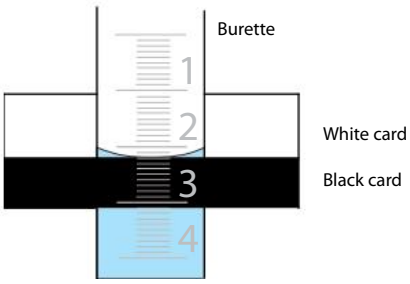

Figure 214 A burette reader

The Volumetric Flask

This should be rinsed with distilled water before use. If you are dissolving an accurately weighed solid sample you must ensure that all the sample is transferred to the flask. One way to do this is to transfer the solid from the weighing bottle to a clean beaker. Wash the weighing bottle at least three times with distilled water, adding the washings to the beaker. Now add enough water to dissolve the solid and warm the solution if necessary. Cool and transfer the solution to the volumetric flask using a small funnel. Wash the beaker and funnel several times with distilled water adding the washings to the volumetric flask. Now make up to the mark with distilled water. Add the water in drops when close to the mark. Stopper the flask and invert several times so the resulting air bubbles ensure thorough mixing of the solution.

Graduated glassware should never be heated, otherwise the glass expands and the scale or mark loses some accuracy. Ideally, the flask should be filled at 20 °C, or the temperature that is recommended by the manufacturer.

Weighing can be done by difference, for example,

Mass of weighing bottle and anhydrous sodium carbonate	= 11.045 ± 0.001 g
Mass of weighing bottle and residual solid	= 10.155 ± 0.001 g
Therefore, mass of anhydrous sodium carbonate used	= 11.045 g – 10.155 g = 0.890 ± 0.002 g

Titration Flask

A conical/Erlenmeyer flask should be used for titrations as the narrow neck reduces the chance of losing any solution through splashing. This should be thoroughly rinsed with distilled after before use and between titrations. During a titration, rinse down splashes on the sides of the flask, with a little distilled water from a wash bottle.

During the actual titration, the conical/Erlenmeyer flask should be placed on a white ceramic tile and it should be held close to the burette to minimise losses by splashing. The contents of the flask should be continuously swirled to avoid any local build up of reagent added from the burette.

If a burette with a tap is being used, then the tap may be held in the left hand (if you are right handed) and the flask in the right hand. As the end-point is approached, transient or temporary colour changes occur in the flask that hint at the colour of the indicator at the end point.

The titration should be continued with the slow addition of the chemical from the burette one drop at a time until the end-point is reached, then:

1. The solution changes colour, if a two-colour indicator is used for example, methyl orange or bromothymol blue;

or

2. The solution is decolourised or colourised if a one-colour indicator is used, for example phenolphthalein. The intensity of phenolphthalein is determined not only by the pH of the solution but also by the total amount of indicator (provided the pH is $pK_a \pm 1$).

If you are unsure whether the colour has changed, record the reading and add one or more drops of the reagent from the burette to see if there is a noticeable difference. The colour of the indicator before and at the end point should be recorded. The colour at the end point should be maintained for at least thirty seconds. A trial titration is often useful so that the end point can be approached rapidly and carefully in subsequent titrations.

A number of these titrations (see Table) should be performed until you obtain consistent results (i.e. ones which agree to within 0.1 cm^3, since the titration volumes are taken from the difference of two readings each: hence add absolute uncertainties. The conical flask should be washed out thoroughly after each titration.

For example see *Figure 215*.

	Titration Readings		
Titration Number	TRIAL	1	2
Second Burette Reading /cm^3	(24.20)	48.10 ± 0.05	23.90 ± 0.05
First Burette Reading /cm^3	(0.00)	24.20 ± 0.05	0.00 ± 0.05
Titre Volume /cm^3	(24.20)	23.90 ± 0.10	23.90 ± 0.10

Figure 215 Sample titration data

The two accurate titrations are both 23.90 ±0.10 cm^3.

If, however, the spread of values that you are averaging is greater than 0.1 cm^3 then the systematic errors of your titration are greater than the random errors inherent in the experiment. This error could be estimated to be half the spread of the averaged values. Use whatever value is greater, but you do not need to add the errors.

Balances

The Use and Misuse of Balances

Weighing is one of the most fundamental procedures performed in the laboratory and can create all manner of problems during quantitative practical work if not carried out properly. The following list describes several weighing techniques and procedures that should be avoided and how they can lead to errors.

Weighing hot samples

This will generate an upward convection of warm air that will cause an upward force to be applied to the balance pan. The result will be an apparent mass that is less than the actual mass. In the case of a weighing, the final result will appear lower than the actual value.

Weighing materials that lose water rapidly or are extremely hygroscopic on an open balance pan or in an open vessel.

The loss or gain of water during weighing will give false low or high masses. Always weigh wet or hygroscopic materials in a closed container such as a covered weighing bottle.

Weighing objects that are too large for the balance pan or weighing off-centre.

This can cause instability and buoyancy effects resulting in variable and unpredictable results.

Weighing volatile liquids in an open vessel.

The weight will continually decrease due to loss of sample by evaporation. As a result the mass recorded will be greater than the true mass because of further evaporation between the time the weight is recorded and when the sample is transferred and diluted with a suitable solvent.

Sample is spilled on a balance pan.

If this is not noticed, then the amount of sample actually being used in the analysis will be less than the recorded mass. The recorded mass will be low. Always make sure the balance pan is clean before and after using a balance.

Forgetting to weigh the stopper

Consider taring (calibrating the balance to zero) a stoppered volumetric flask on a balance pan, removing the flask, transferring a liquid sample into the flask, and then reweighing the flask plus the sample without the stopper. This is easily recognised by an unexpectedly low or negative sample mass.

Open balance doors

Drafts and air currents will cause weighing uncertainties and inaccuracies in analytical results.

Excessive vibration

If a balance is not on a surface that is vibration free, then accurate balance readings will be impossible to record.

Weighing on a balance that is out of calibration, out of level or not properly damped

Weighing performed on a balance that is past its calibration due date cannot be considered reliable. Accuracy may also be affected when a balance is not level. Improper damping affects balance sensitivity because a balance that is underdamped will fluctuate to the point where a steady reading is difficult or impossible to obtain. Overdamping, on the other hand, will inhibit a balance from responding quickly enough to changes in weight as a sample is applied to the balance pan. The results may then lack accuracy.

Spectrophotometers and Colorimeters

These instruments are most sensitive if the light falling on the solution under investigation corresponds to the range of wavelengths actually absorbed by the substance. The difference between the solvent and the solution is then greater, and the absorbance reading higher. Errors due to wavelength drift and the finite bandwidth of wavelengths selected by the monochromator are minimised because the spectrum varies least with wavelength at the absorbance maximum.

It is therefore important to select the appropriate range of wavelengths. In colorimeters this is achieved by placing a colour filter in the path of the machine's light beam. The colour of the filter should be complementary to the colour of the solution under investigation. The colour wheel in *Figure 216* will help in choosing a suitable filter.

The scale of a spectrophotometer is shown in *Figure 217*. Note that the absorbance is a logarithmic scale and % transmittance is a linear scale. The absorbance reading shown is 0.234, but the last figure, 4, is an estimate.

The transmittance is 58.3%. Note that because the transmittance scale is smaller than the absorbance scale, at this point, there is more uncertainty in the last digit of transmittance.

The transmittance may be quoted as 58.3 ± 0.2%.

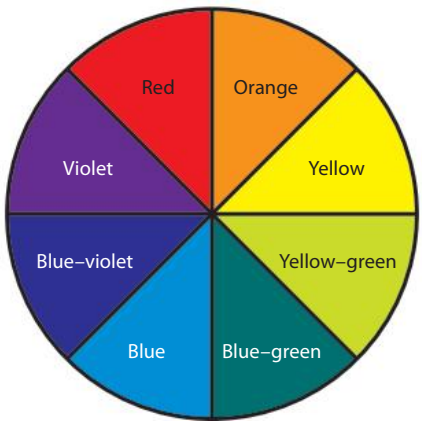

Figure 216 Colour wheel

For example, an orange filter should be chosen if an aqueous solution of copper(II) sulfate, which is blue in colour, is under investigation. If the solution is not strongly coloured a 'trial and error' process can be carried out. Try each filter to find out which one gives the maximum absorbance.

Since an instrument of this type may 'drift' (leading to random errors), it is important (time permitting) to re-check the zero reading with your 'blank' (usually distilled water) before each measurement is made.

Since the temperature of the cell compartment is generally several degrees higher than the surrounding room temperature, it is important to remove the cell containing the reaction mixture immediately after a measurement has been taken.

All vessels should be covered to protect them from dust, which scatters light and therefore makes it look like the absorbance of the sample has increased. Cuvettes should be handled by the sides that the light will not be passing through (usually opaque or ridged) to avoid placing fingerprints on the optical faces, which must be kept clean to avoid surface contamination, which also leads to scattering.

It is also important to place a cuvette in the machine as reproducibly as possible. A slight misplacement of the cuvette in its holder, or turning a flat cuvette round by one hundred and eighty degrees, or rotation of a circular cuvette, all lead to random errors in absorbance measurements.

These instruments are probably most accurate when measuring absorbances of around 0.5 to 1.0. The scale may tend to become slightly non-linear with absorbance in the region 1.5 to 2.0, when the intensity of the transmitted light is very low, because under these conditions the response of the photo-detectors may no longer be linear and stray light becomes significant. See *Figure 217*.

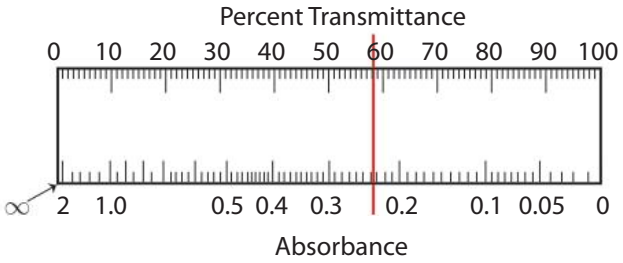

Figure 217 Scale of a spectrophotometer

Conversely, if too much light leaves the sample (low absorbance) because of its low concentration of solute, it is difficult for the machine to distinguish the transmittance of the sample from that of the reference.

pH Meter (glass electrode type)

Take care to clean the electrode thoroughly by rinsing it with distilled water from a wash bottle every time you change solutions. Do not leave the electrode un-immersed for longer than you need, or let the electrode dry out: salt deposits will form interfering with the electrode response.

Standardise the meter (see *Figure 215*) (as in the instructions or demonstrated by your IB Chemistry teacher) at a particular pH and temperature using the buffer(s) provided. The buffer solutions provided must be made up with care since the accuracy of your pH measurements will depend on the accuracy of the buffer solutions used in calibrating the probe.

The buffer provided should reflect the nature of solutions whose pH values you are going to measure. For example, if you are investigating acidic solutions then an acidic buffer solution (e.g., pH 4.0) should be provided. The measurements would be a little less accurate should a neutral (pH 7.0) or alkaline buffer solution (e.g., pH 9.0) be used. Check to ensure that the buffer solutions have not 'expired'.

Figure 218 shows a pH METER *(manufactured by Hanna Instruments) (Photograph by Robert Balcer, formerly of Overseas Family School, Singapore)*

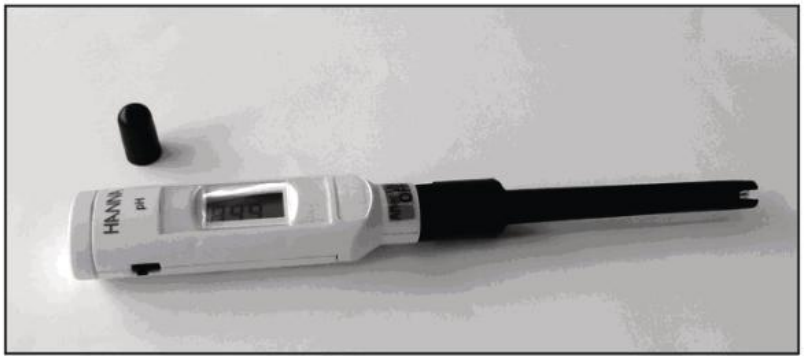

Figure 218 shows a pH meter

However, calibrating with two buffers allows the 'slope' of the pH meter to be set so that it reads correctly at all pH values. Attention to the following points will enable you to obtain the highest accuracy:

Do not touch the electrode or move about near it whilst a reading is taken. If you are using a magnetic stirrer then switch it off when you take the readings.

The electrode needs time to reach equilibrium in solution, so do not rush to record the measurement, but wait patiently until the meter reading becomes steady.

If the meter is not steady, try to establish whether, over a period of a minute or so, it is:

- approaching a steady reading exponentially.
- oscillating regularly about a mean value.
- drifting continuously in one direction.

If one of these patterns can be identified then you should be able to decide the best way to record accurate readings and an appropriate uncertainty for your particular meter in a consistent way. This might be to wait one minute before taking the reading, to average the high and low points of the oscillation, or to take the reading immediately.

pH meters actually measure - $\log_{10}$ [activity of hydrogen ions]. At high concentrations, ions interact with each other, so that their effective concentration is reduced. Consequently, pH meters tend to record higher values than you would expect for concentrated solutions.

It may be possible for you to connect your pH meter and probe to a personal computer to record a series of pH measurements over a period of time

Extracting and Studying Enzymes

In some of the Topics you are likely to perform some experiments involving plant or animal enzymes. The main features of such experiments are the difficulties associated with delicate and sensitive biological materials.

The enzymes may be supplied in a purified form or you may have to extract them from fresh plant materials. A common approach involves grinding up the materials in a pestle and mortar, with a little fine sand to break down the cellulose cell walls. For particularly tough plant tissues a food blender or food processor may be used for short periods of time.

Enzymes are very sensitive to changes in pH, the polarity of the solvent, the presence of dissolved salts and temperature. The crude (impure) extracts of enzyme are therefore placed into a buffer solution of specified pH. To minimise enzyme degradation the crude enzyme extract is kept cool at all times, from extraction, through filtration to final use.

Enzyme activities will often decrease as the enzyme solution stands, even if stored in a refrigerator, hence experiments involving enzymes must be performed relatively quickly on the same day.

Handling Gases

During your IB Chemistry Practical Programme you may have to collect gases for testing, or to measure the volumes released during kinetics or stoichiometry investigations.

Collecting Gases

The method used will depend on whether the gas is soluble in water. If it is soluble the gas will have to be collected directly in a gas jar (see *Figure 219*). If the gas is insoluble in water it can be collected over water in a test tube or measuring cylinder (see *Figure 220*).

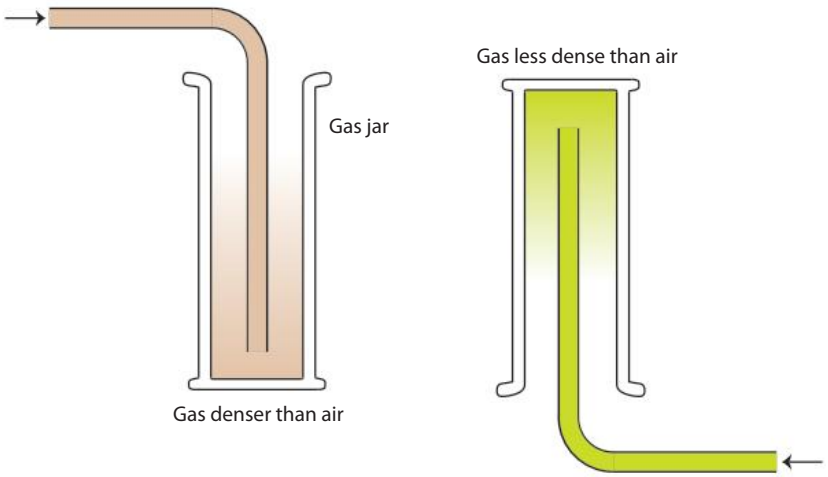

Figure 219 Collecting gases by displacement of air

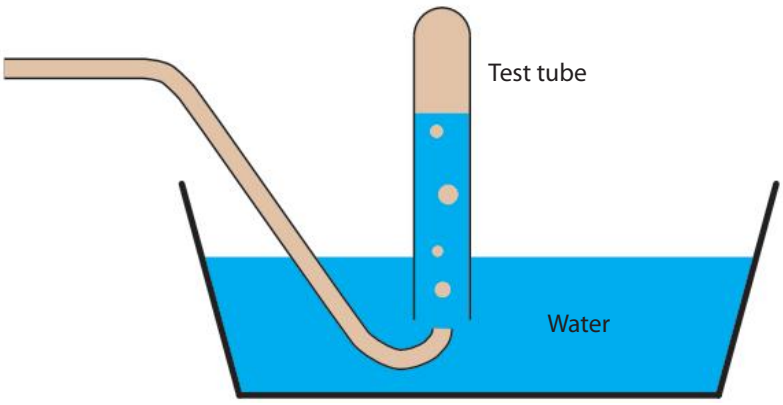

Figure 220 Collecting insoluble gases over water

Measuring Volumes of Gases

The gas can be collected over water in an inverted burette or in a gas syringe (see *Figures 221 (a) and (b)*). Before you commence any experimental work ensure that the system is airtight and check that the rubber or plastic tubing fits tightly. Do not clamp the syringe too tightly since this will prevent the gas from pushing the inner section freely.

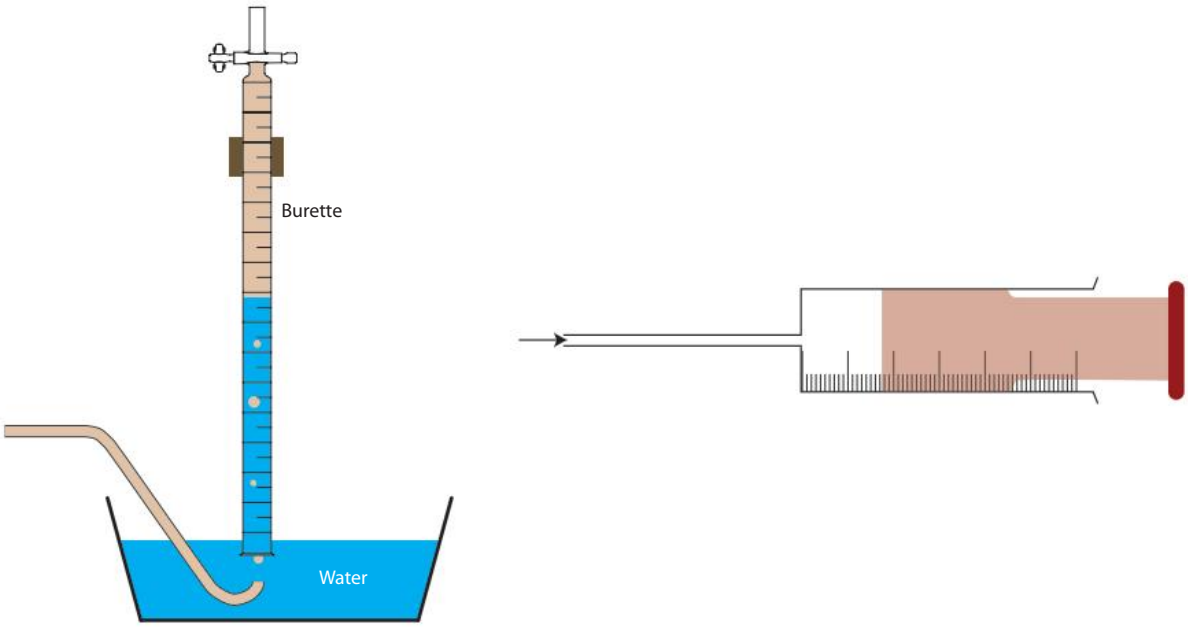

Figure 221 (a) and (b) Techniques for ollecting and measuring volumes of gases

Washing and drying gases

A gas washing bottle can be used. For example, if a gas is contaminated by acid it can be 'washed' or 'scrubbed' by bubbling it through aqueous sodium hydroxide which neutralises the acid. The commonest way of drying gases is to bubble through them concentrated sulfuric acid which removes the water vapour from the gas (*Figure 222*). You must consult your IB Chemistry teacher or instructor before using concentrated sulfuric acid.

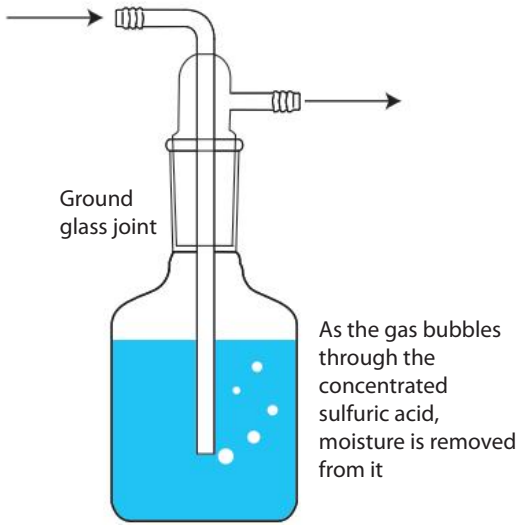

Figure 222 Drying gases

Constructing Simple Electrochemical Cells

An electrochemical or galvanic cell is set up so that the two redox reactions (described by half equations) are separated in space. Each electrode is immersed in aqueous solution in a small beaker. The two solutions of metal ions are linked by a salt bridge which allows the movement of ions in both directions and the electrodes are connected via wires forming an external circuit, around which electrons flow.

To determine the maximum potential difference or voltage that can be generated between the electrodes, a high-resistance voltmeter is connected to the external circuit. A high-resistance voltmeter is required so that very little current is drawn from the circuit.

Several precautions are needed to ensure accurate values of cell potentials are obtained:

- The surface of the electrodes must be thoroughly cleaned with carborundum (silicon carbide) or 'wet-and-dry' paper to ensure any unreactive metal oxide layers are removed. The electrodes should then be washed with distilled water and dried. To ensure they are grease-free they should be rubbed with cotton soaked in propanone (acetone) before a final rinsing. The cleaned electrodes should now only be handled by tweezers at the edges. This cleaning process is particularly important if relatively reactive metals like magnesium are used. Magnesium will not be able to reach the thermodynamic equilibrium potentials because of the competing hydrogen evolution reaction that takes place from the reduction of water.
- A good electrical contact is needed between the electrodes and the external circuit. Clean rust-free crocodile clips must be used to minimise the resistance introduced into the circuit. The circuit should then be completed with a salt bridge–this normally takes the form of a piece of filter paper dipped in saturated aqueous potassium nitrate solution. Potassium chloride can also be used, unless silver ions are present in one of the half cells: when insoluble silver chloride would be precipitated. Salt bridges should be left in the solutions for the minimum time in order to reduce contamination. A high-resistance voltmeter should then be connected between the electrodes and the potential difference or voltage measured and recorded. If the voltmeter is a digital voltmeter and gives a negative reading, or if with an analogue meter the needle moves below zero, then the voltmeter needs to be connected the other way round to get a positive reading.

Measuring Molar Masses of Gases

The simplest method for determining the molar mass of a gas is via direct weighing: a flask is weighed empty, that is, full of air; the flask is then weighed full of gas and then finally the flask is weighed full of water. An appropriate sized measuring cylinder is then used to determine the volume of water, that is, the volume of the flask.

It is not a good approach to measure the volume of the flask at the beginning of the experiment since the drying of the flask will be a time consuming process. If the flask is not dried properly and is damp, then the gas used may dissolve in the remaining water droplets, thus leading to an error in the measurement of the volume of gas contained in the flask.

Another error inherent in this approach is that some water remains in the flask when its volume is determined. This is unavoidable, but introduces a systematic error into the experiment.

Some gases, especially hydrogen chloride, sulfur dioxide and ammonia are very soluble in water. The molar masses of these gases can be determined using an experimental approach similar to the one just described. A flask is weighed empty (that is, full of air), then the gas is passed into it for a short period of time before the tubes are then sealed and the flask and contents reweighed.

One of the tubes leading into the flask is opened under water and owing to the solubility of the gas, the pressure inside the flask is reduced and air pressure pushes water into it, but once all the gas has dissolved, no more water enters the flask. The amount of water that did enter is measured by pouring it into a measuring cylinder of an appropriate size. Finally, the volume of the flask is found by filling it completely with water.

It is common for this type of experiment to overestimate the molar mass of the gas under investigation. This occurs, in part, because not all the water is transferred from the flask to the measuring cylinder – a so-called mechanical loss. This underestimates the volume of the gas, thus leading to a higher calculated molar mass.

It is important to dry the flask and tubing thoroughly before they are used in the experiment, otherwise the gas will dissolve and react with the moisture. This will increase the mass of gas in the apparatus, but it will add negligible volume. Therefore the molar mass of the gas will be overestimated. Another source of error is the non-ideal behaviour of these gases.

Measuring Equilibrium Constants

To measure a chemical equilibrium constant, K_c the following issues need to be taken into account:

- The reactants and products of the reaction must have actually reached chemical equilibrium. You can test if this has happened by removing small samples out of the reaction mixture at different times and analysing them. When identical concentrations are obtained for successive analyses, then you can assume that equilibrium has been achieved.
- It may also be possible to analyse the system without physically removing samples. For example, depending on the reaction under study, a colorimeter may be used.
- Equilibrium constants should only be measured for systems where the concentrations of the chemical species are relatively low. At high concentrations interactions occur between the particles and substances in a mixture may behave as if their concentration were less than its real value due to molecular or ionic interactions. Hence, you are not be justified in calculating experimental equilibrium constants to more than two significant figures.
- The temperature at which the measurements are performed must be known and kept constant. Equilibrium constants vary with temperature and are quoted for specific temperatures. This is usually achieved by performing the reactions in a water bath whose temperature is kept constant using a thermostat.
- The concentrations for gases must be found. The most common approach to measure concentration of water soluble gases is by performing an acid-base or redox titration. The reaction mixture should be quenched in cold water to slow the reaction down. The solutions of the gases are then analysed by a direct titration or by a back titration. Datalogging probes can also be employed, for example, a dissolved oxygen probe.

For example, the quantity of sulfur dioxide can be determined by reacting it with hydrogen peroxide and titrating the sulfuric acid formed with standardised alkali.

$$SO_2\,(g) + H_2O_2\,(aq) \rightleftharpoons H_2SO_4\,(aq)$$

Ammonia gas can be reacted with an excess of dilute hydrochloric acid. The resulting solution can be made alkaline, heated and the ammonia liberated is dissolved in a large excess of hydrochloric acid. The acid is then back titrated with standardised sodium hydroxide.

Common Organic Chemistry Practical Techniques

Glassware with interchangeable ground glass joints (refluxing and distillation)

The joints should be greased only lightly: excessive grease is difficult to remove and leaves the glass looking dirty and may contaminate the product. A suitable building point for your apparatus is normally the reaction flask. Try to use and the minimum number of clamp stands and bosses to hold your apparatus in place. A Liebig condenser is best secured by a clamp to the same retort stand as that holding the flask. This will require the use of a variable boss which can be set an appropriate angle. Such an arrangement will avoid the condenser separating slightly from the rest of the refluxing or distillation apparatus. You will also find it easier to move your apparatus around if only one retort stand is used.

Refluxing

Many organic reactions are relatively slow and their reaction mixtures need to be kept hot for significant lengths of time. In addition, many of the organic liquids used as either reactants or solvents are volatile, flammable and toxic. Some organic reactions may also produced volatile liquids or gases.

All of these problems can be overcome using a technique called refluxing (see *Figure 223*). It involves fitting a Liebig condenser to the top of the reaction flask. Cold water is then passed through the outer jacket of the condenser. When the contents of the flask are heated, the organic liquid will boil and the vapour will rise up inside the condenser. There it meets the cold walls of the condenser where it is cooled below its boiling point and condenses back to a liquid. This then drips down the walls of the condenser and is returned by gravity to the reaction mixture in the flask.

To ensure smooth boiling anti bumping granules–in the form of very fine pure sand–are placed into the flask prior to refluxing. Often the heating is carried out in a water bath or a steam bath, rather than heating directly with a Bunsen burner. This is done if any of the organic products or reactants are especially volatile and flammable, or if the reaction mixture must not be allowed to rise above 100 °C.

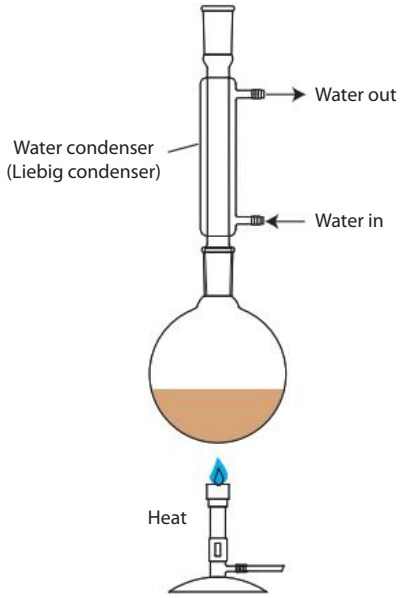

Figure 223 Heating under reflux

Recrystallisation

Recrystallisation is a valuable technique for purifying the impure solid product obtained from a reaction, typically an organic reaction. The substance to be purified is dissolved in a solvent that dissolves more solute when it is hot than when it is cold. A suitable solvent can be found by a process of 'trial-and-error' or by consulting an appropriate organic text. For many organic solids ethanol is used.

The aim is to use just enough solvent to dissolve the solid when the mixture is hot. This will enable the maximum amount to crystallise on cooling (the use of ice may be necessary). Some solids with low melting points may form an oil. If this occurs, you will need to add more solvent until the oil has been dissolved. Check that the solution does not contain any insoluble solid impurities, for examples particles of carbon (frequently formed during organic reactions by a so-called 'charring process'), if it does it will need filtering through a pre-heated funnel. This filtration can be carried out using one of two methods: a filter funnel, conical flask and 'fluted' filter paper or a Büchner flask and funnel. The fluted filter paper increases the surface area for filtration so that filtration is rapid. If it is not rapid then the solvent will cool down and the product may crystallise out in the filter paper.

Leave the hot solution to cool slowly and undisturbed. Occasionally supercooling occurs and no crystals form; the solution is said to be supersaturated. If this occurs shaking the flask may be all that is required to start rapid crystallisation. Alternatively, scratching the side with a glass rod (to release tiny crystals of glass) or, if available, a small seed crystal of the pure solid, may initiate crystallisation.

When the pure product has crystallised out, leaving soluble impurities in solution, filter off the crystals using a clean, dry Büchner funnel and flask. Wash the product with a minimum of cold solvent to remove any solution adhering to it, and then dry by drawing air through the crystals to evaporate most of the solvent and finally in a dessicator.

Determination of boiling point

There are two methods which can be used to measure the boiling point of a liquid. The first involves simple distillation and a relatively large volume of the liquid (see *Figure 224*). A flask is half-filled with the organic liquid and a few anti-bumping granules to ensure the liquid does not 'bump' and boil explosively. The apparatus for simple distillation is then assembled and the bulb of the thermometer placed at the entrance to the condenser. The boiling point of the liquid is the steady temperature shown as the liquid distils over.

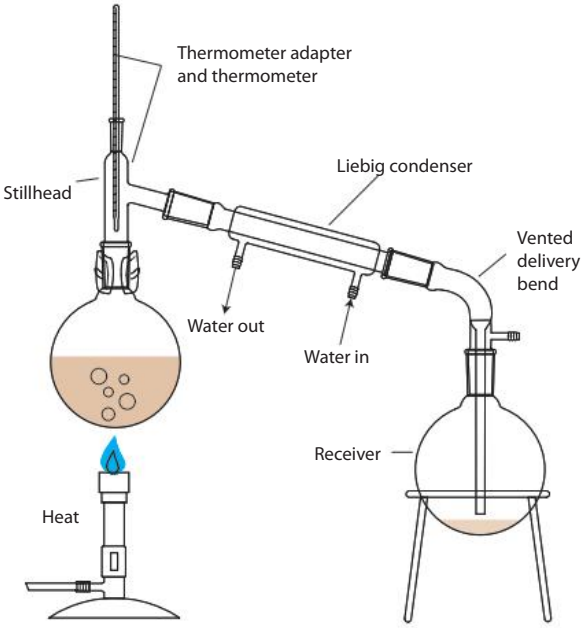

Figure 224 Simple distillation to determine the boiling point of an organic liquid

The second method of determining boiling points is known as the *Siwoloboff* method (*Figure 225*) and is applicable to both pure liquids and mixtures of liquids (they would be separated by distillation). It also can be used with relatively small volumes of liquid.

The technique is based upon the principle that the boiling point of a liquid is temperature at which the vapour pressure of the liquid is equal to atmospheric pressure. A small volume of the organic liquid is placed into a small ignition tube into which is placed a capillary tube, sealed at one end, open end down. The tube is attached to a thermometer and placed in a beaker filled with a high boiling point oil or water. The oil or water are heated very slowly and stirring is carried out to ensure the heat is evenly distributed.

Heating is stopped when a rapid and continuous stream of bubbles emerges from the capillary tube. The temperature is noted when the bubbling has stopped and the organic liquid appears about to be sucked up into the capillary.

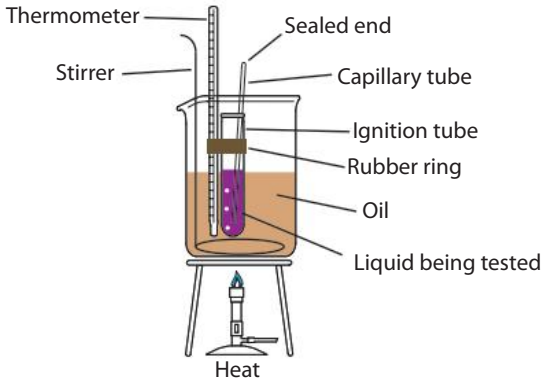

Figure 225 The Siwoloboff method to determine the boiling point of an organic liquid

This is the boiling point of the liquid. This is because at the boiling point the pressure of the vapour of the liquid in the capillary tube is just overcome by the atmospheric pressure (one atmosphere), and the liquid is pushed back into the capillary tube.

Büchner or Suction Filtration

To set up the funnel for filtration, a filter paper with a similar diameter to the flat bottom of the funnel is needed. If necessary, but less preferably, a large filter paper can be cut to size. The filter paper is then moistened with a few drops of the solvent used in the solution to be filtered. The flask is connected to a pump and the funnel placed in the rubber cone. It may be necessary to press down on the funnel to help it seal with the rubber. It also helps to clamp the Büchner flask. If the filter paper tears under the pressure developed by the pump, then place two filter papers on top of each other. The mixture to be filtered in then directed on to the centre of the filter paper by slowly pouring it down a glass rod, whilst suction is applied by the pump. Before doing this swirl the mixture so that crystals are carried into the funnel. It may be necessary to scrape out the remaining crystals into the Büchner funnel using a glass rod. Alternatively, some of the filtrate may be returned to the flask containing the crystals to help wash them all out.

Determination of a melting point

The melting point of an organic solid will give some indication of the purity of the substance. Pure solids have 'sharp' melting points and melt over a narrow range of temperatures. The melting point of a solid can also help determine the identity of an organic substance, either directly, or indirectly, through the melting point of a derivative

The sample for the melting point determination should be dry and crystalline. It should then be ground to a fine powder using a clean, dry pestle and mortar. Some of the sample should be introduced into the melting point tube. You need sufficient sample to view clearly. Using the ridged edge of a coin may help to vibrate the melting point tube and allow the solid to fall to the bottom of the tube.

The sample is observed closely and the temperature over which melting starts and ends noted. Repeat the melting point determination with a fresh sample and approach the melting point with a very slow increase in temperature. If the substance is recrystallised again, it is likely to have a slightly higher, sharper melting point. This is because impurities have the effect of lowering the melting point (by reducing the intermolecular forces within the lattice) and making it less sharp, that is, broader.

The simplest form of melting point apparatus are boiling or Thiele tubes filled with a high boiling point oil (*see Figure 226*). The capillary tube with its sample is attached to a suitable thermometer. The oil is then heated and the crystals carefully observed until melting begins. The temperatures over which melting occurs is recorded.

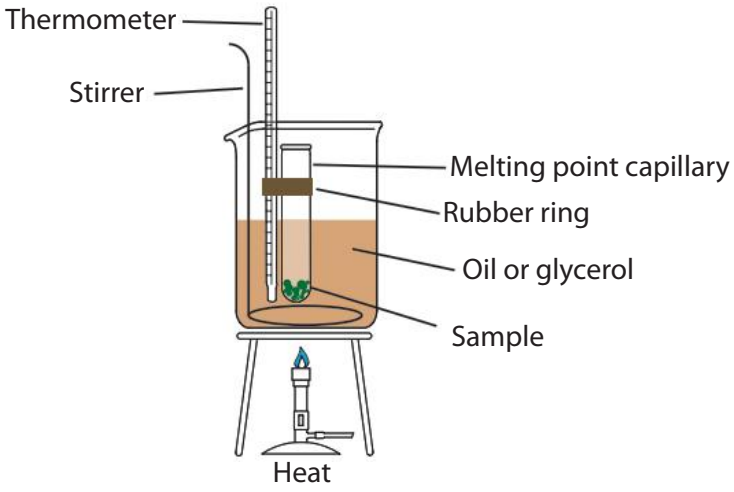

Figure 226 Simple melting point apparatus

Melting point determinations are best performed in an electrical melting point apparatus. The melting point tube and thermometer are placed into holes located in a large block of high resistance metal which is heated electrically. The crystals are observed through a magnifying glass and the temperature of the block is raised until the crystals begin to melt.

Drying liquids

A liquid organic product may require drying before a final separation by distillation. A small quantity of the drying agent (typically anhydrous calcium chloride or anhydrous magnesium, sodium or calcium sulfates) is added to the solution in a suitable stoppered flask. The mixture is swirled and allowed to stand before filtering, preferably using a small plug of wool to remove the excess drying agent.

Use of a separating funnel

Preparing a pure organic liquid involves several stages. After refluxing and distillation, the product will be present in a mixture which may contain water, unreacted reagents and a variety of side products. Further purification of organic liquids often involves the use of an immiscible solvent in which the product is more soluble than the impurities and this can be separated off using a separating funnel.

Ensure that that the ground glass joints are lightly greased and the tap of the separating funnel is securely closed. The mixture of solvents is placed in the separating funnel–ensure the tap is not leaking. The funnel is stoppered and the stopper held firmly in place with a forefinger and the funnel inverted (turned upside down). Any pressure build-up may be released through the tap while the funnel is inverted. The separating funnel is now placed in a clamp stand and the contents allowed to settle, a process which may take several minutes. Remove the stopper and drain the lower layer (the one with the lower density) into a clean flask. Close the tap so that the meniscus between the two layers is caught in the tap. If the upper layer is required this is poured out of the top of the funnel. This avoids contamination with the last trace of lower liquid in the tap.

Distillation

Simple distillation is frequently used during organic synthesis to separate the desired organic product from a reaction mixture that may contain less volatile liquids, or occasionally organic solids or involatile inorganic solids (for example sodium bromide used to prepare hydrogen bromide *in situ*).

The technique, which employs the apparatus previously shown in *Figure 226*, is based on differences in boiling points and is most efficient when there is a relatively large difference in boiling point between the components of the reaction mixture.

The thermometer bulb is placed in the side arm adaptor so the bulb is located at the entrance to the condenser. It records the temperature of the vapour as it 'distills over' into the condenser, this is the boiling point of the distillate.

The heating of the reaction flask is adjusted so that the distillate is being collected at a steady slow rate. The temperature will remain constant while a particular product is distilling over. Liquids with higher boiling points and involatile solids remain in the flask. To promote smooth boiling some anti-bumping granules should be placed in the flask with the liquid.

The process of separating of two or more volatile liquids is improved if fractional distillation (see *Figure 227*) is employed. In this technique a long column filled with inert glass beads is placed between the flask and the side arm adaptor.

Before you perform a distillation you need to have an idea of the fractions that you are likely to obtain, for example, solvent, pure product, starting reagent etc. and you should, if possible, know their boiling points. You should have several labelled flasks ready to receive these fractions. You will notice that the temperature remains steady while one product is distilling over.

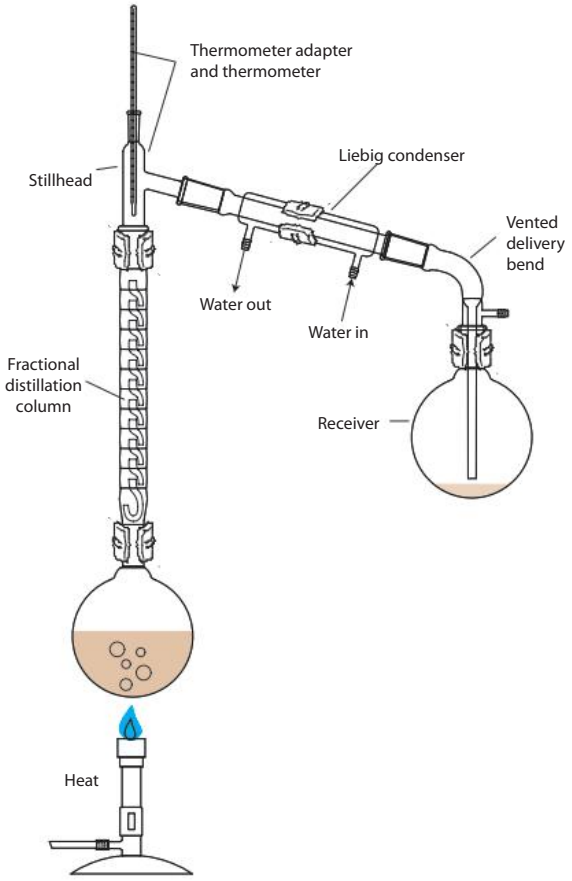

Figure 227 Apparatus for fractional distillation

Calorimetry

Calorimetry is the name given to the experimental technique used to determine the heat energy absorbed or released during a chemical reaction.

Calorimetry experiments can be performed using a polystyrene cup and a thermometer. This simple apparatus can be used to investigate enthalpy changes for a wide variety of reactions involving aqueous solutions, for example, enthalpies of replacement and neutralisation.

The heat energy released when a fuel burns, for example, an alcohol, can also be determined using a similar procedure. A 'spirit' burner containing a liquid fuel is placed under the copper can (which acts a calorimeter) containing a known volume of water. *Figure 228* shows a simple apparatus for measuring the enthalpy change of combustion of a liquid fuel.

The initial temperature, the mass of the water and the initial mass of the spirit burner are measured before the start. The wick is then lit and the heat produced as the fuel burns is used to heat the water in the copper can. After a suitable period of time, the flame is extinguished, the lamp reweighed and the final temperature of the water recorded. However, this simple apparatus suffers from significant heat losses.

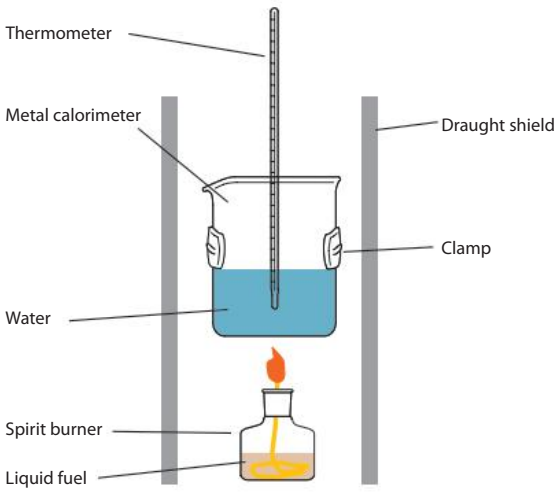

Figure 228 A simple calorimeter

The apparatus in *Figure 229* is designed to overcome some of the problems associated with heat losses and will therefore allow more accurate values to be obtained for enthalpies of combustion. The spirit burner is surrounded by water jacket, which helps to prevent draughts and ensures a more efficient transfer of heat from the flame to the water. The warm gases produced during combustion, namely, steam and carbon dioxide, are drawn through the apparatus using a water pump, and heat energy is transferred to the water via a copper coil.

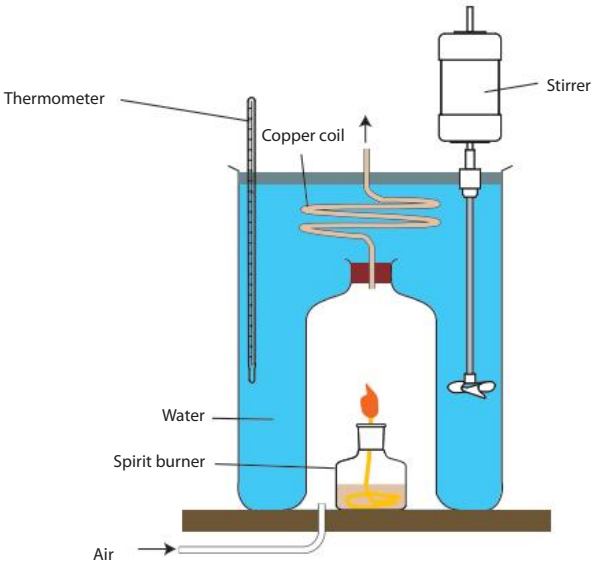

Figure 229 A (flame) combustion calorimeter

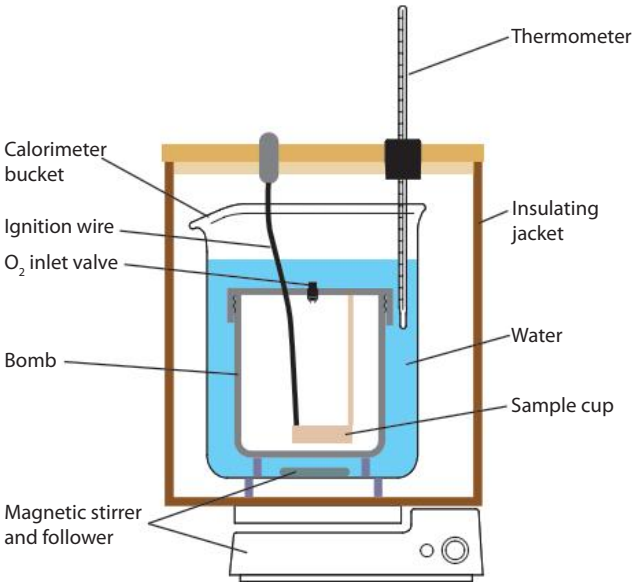

Figure 230 The bomb calorimeter

However, some heat energy is used to warm the glass and copper from which the calorimeter is constructed. The apparatus is therefore normally 'calibrated', by burning a fuel of known enthalpy of combustion over the same temperature range as used for the unknown fuel.

One drawback with this calorimeter is that some of the fuel may undergo incomplete combustion, resulting in an error. The most accurate measurements of enthalpies of combustion are obtained by the use of a bomb calorimeter (see *Figure 230*).

A weighed sample of the substance to be burnt is placed in a steel 'bomb' capable of withstanding large increases in pressure. The bomb is filled with oxygen, sealed and the surrounded by water. After the initial temperature of the water has been recorded, the contents of the bomb are ignited electrically. The heat produced during the combustion reaction is transferred to the water surrounding the bomb and the final temperature recorded. Calibration is required, using a known amount of energy (usually found from the electrical energy required to give a similar temperature rise) to determine the heat capacity of the calorimeter. This gives the internal energy change (that is the heat change at constant volume) rather than the enthalpy change (which refers to constant pressure), though one can be calculated from the other.

Experiments involving Electricity

In investigations involving electrolysis or electrochemical cells you will need to connect circuits using a circuit diagram or you may have to construct your own circuits if the investigation involves the Exploration criterion.

Connecting an Ammeter and a Voltmeter

An ammeter is connected in series with the device, whilst the voltmeter is connected in parallel. The terminals of the ammeter and the voltmeter have a polarity. They need to be connected to the right poles of the power source. The red terminal is positive while the black terminal is negative. To work properly, the positive terminal of the ammeter or of the voltmeter must be connected to the positive side of the power source. Refer to *Figure 231*.

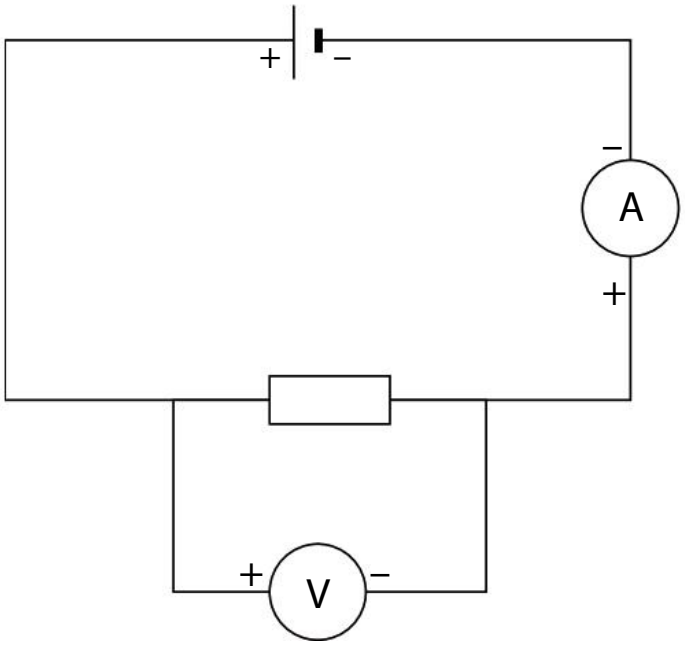

Figure 231 Circuit diagram showing the correct connection of a voltmeter and an ammeter

Listed in Figure 232 is a summary of what you need to do to score well in the Exploration criterion.

Assessment criteria	Evidence required	What you must do
Identifies a topic, a relevant and fully focused Research Question is clearly described. Relevant and appropriate background information is provided to increase the understanding of the context of the investigation	A topic, a relevant and fully focused Research Question are described	Identify the topic and state the Research Question, for example: The investigation will determine how the 'independent variable' affects the 'dependent variable'. The following will be kept constant: controlled variable 1, controlled variable 2,… and the method for measuring the dependent variable.
	Relevant and appropriate chemical background is included	Give relevant background information including a summary of the chemical literature and a testable hypothesis and perhaps reference to a relevant chemical model or chemical theory and identifies the main chemical processes involved and the likely causes at the molecular, atomic or ionic level. Makes quantitative predictions in words and in the form of graph. (*Where appropriate*)
	State the relevant variables explicitly	Classifies and tabulates key variables. • Independent variable (one only) • Dependent variable (one only) • Processed variables (one or more) • Controlled variables (typically more than one) • Identify variables over which little control can be exerted
Designs a methodology that allows relevant, reliable and sufficient data to be collected. Shows full awareness of safety, ethical and environmental issues	Appropriate choice of chemicals, materials and apparatus	List of all chemicals (physical states, purity, volumes and concentrations) (where appropriate)) and apparatus and instrumentation (state manufacturer (where appropriate)) with specifications including precision/random uncertainty. A labelled and cross-sectional diagram of any set-up of apparatus with a justification and explanation for the methodology.
	Effective control and manipulation of variables	A clear description of the method which • describes how the independent variable is to be varied and measured accurately • describes how the dependent variable is measured • includes a logical sequence of steps to be taken and their rationale • includes details of any modification or adaptations of standard methods and justification for their use • includes a clear account of how and why the controlled variables are kept constant. • includes a statement of how the plan will produce relevant, reliable and sufficient results. • includes a statement of how the plan will produce accurate and precise results. • draws up bank results tables and graph axes and describes how the raw data will be processed • includes where appropriate, an explanation of the chemical and physical principles behind your plan. • includes control experiments should be described (if relevant) • includes a detailed statement of how the plan ensures an ethical and safe investigation (risk assessment) that minimises the impact on the environment. • describes safety precautions taken to keep risks to a minimum • describes how chemicals are to be disposed of and stored
	Appropriate number and range of readings to be taken	State you will take measurements for at least five values of the independent variable. Also consider what the reading at zero will be. State the range of values for the independent variable i.e. the lowest and highest values and the size of the increment. State the number of repetitions for each value of the independent variable.

Figure 232 Summary of the Exploration criterion

This criterion assesses the extent to which the student's report provides evidence that the student has selected, recorded, processed and **interpreted** the data in ways that are relevant to the research question and can support a conclusion.

The following table is an extract from the IB Chemistry Guide and is the basis that will be used by your teacher and the moderator for the assessment of your work.

MARK	DESCRIPTOR
0	The student's report does not reach a standard described by the descriptors below.
1-2	The report includes **insufficient relevant** raw data to support a valid conclusion to the research question. Some **basic** data processing is carried out but is either too **inaccurate or too insufficient to lead to a valid** conclusion. The report shows evidence of little consideration of the impact of measurement uncertainty on the analysis. The processed data is incorrectly or insufficiently interpreted so that the conclusion is invalid or very incomplete.
3-4	The report includes relevant but incomplete quantitative and qualitative raw data that could support a simple or partially valid conclusion to the research question. Appropriate and sufficient data processing is carried out that could lead to a broadly valid conclusion but there are significant inaccuracies and inconsistencies in the processing. The report shows evidence of some consideration of the impact of measurement uncertainty on the analysis The processed data is interpreted so that a broadly valid but incomplete or limited conclusion to the research question can be deduced.
5-6	The report includes sufficient relevant quantitative and qualitative raw data that could support a detailed and valid conclusion to the research question. Appropriate and sufficient data processing is carried out with **the accuracy** required to enable a conclusion to the research question to be drawn that is fully **consistent** with the experimental data. The report shows evidence of full and appropriate consideration of the impact of measurement uncertainty on the analysis The processed data is correctly interpreted so that a completely valid and detailed conclusion to the research question can be deduced.

Guiding question:

- *Has the student selected and recorded raw data, including uncertainties and qualitative observations where relevant, that allow for coherent analysis?*

3.1 Data Collection

3.1.1 Recording raw data

Your Individual Investigation will involve your recording qualitative data (observations) and quantitative data (measurements), usually in the form of tables. The tables should have labels in which you briefly describe the contents of the tables and how you recorded the results.

Variables such as time, temperature, concentration, and absorbance of light, which can be read on a scale and which may vary continuously during an investigation, are best arranged in columns. Values can be compared and trends noted more easily than when they are in rows.

The independent variable is written in the left hand column with the dependent variable is written in the right hand column. Processed data is best presented in a separate data table. The number of decimal places should be the same for all values in a column.

Titles, units and the absolute uncertainty (random error) should be given in the headings of the tables, for example, Temperature: T/ °C. If the logarithm, square root, or some other function of a quantity is to represented, the units must appear within the argument, for example, $\ln[p/(\text{N m}^{-2})]$.

You may be recording your raw data by hand in a laboratory note book. You may also be keeping print outs from data-loggers and printed scans from a spectrophotometer. You may also be taking digital photographs of your apparatus and results, such as colour changes during a reaction.

Record **all** your results/raw data–nothing which is observed is 'wrong'. Only after careful assessment should a data point be discarded. When recording data write your observations carefully and completely. Do not use small scraps of paper.

Qualitative observations are just as important as quantitative measurements. Make sure you take note of and record the physical characteristics of substances or solutions involved in the reactions, their colour changes, the evolution of a gas (smell, colour and relative rate of production), whether a solution became hot or colder, etc. Organise these qualitative observations in a separate Data Table or list them in chronological order. For example,

- *"the final colour at the endpoint during titration was a faint pink",*
- *"during the reaction, the bromine water changed from being a bright orange to solution of no colour".*

Report any changes in methodology or unusual conditions.

However, there is a degree of *uncertainty* about the data that result from quantitative measurements. Quantities that are measured directly, such as the volume of a liquid, include errors arising from the limited resolution of the measuring instrument. The calibration of the measuring instrument itself may also lead to systematic errors.

Random errors or random uncertainties should be quantified and recorded with the raw numerical data. Glassware, such as burettes and measuring cylinders, will have the random error or uncertainty printed on the side. Random uncertainties should generally be rounded upwards to one significant figure, for example, record ±0.2 and not ±0.19. The number of decimal places in the data should not exceed the limit of the uncertainty, for example, if the uncertainty is ±0.2 the measurement should only be quoted to 1 decimal place.

Comment on how you arrived at any uncertainty value in the table: the random uncertainty might be derived from a scale, a digital readout or from the manufacturer (see later in section 3.1.3).

Many students tend not to appreciate the need to deal with uncertainty, believing that the process of scientific measurement is unproblematic without any issues. In this incorrect view, measured data points reveal a 'true' value. However, every measurement has its limitations and is susceptible to sources of error.

Systematic errors can result from errors in the calibration of instrumentation. These errors are called systematic because the error is in one direction only, and can therefore be corrected for after data have been collected.

Without observation and measurement, Chemistry and the other Natural Sciences would not exist. In order that Chemical and Scientific theories and hypotheses be developed and tested, it is necessary to record measurements that are accurate, precise, reliable and relevant.

Accuracy is defined as, the ability of a measurement to match the actual value of the quantity being measured. If in reality it is 34.00°C outside and a temperature sensor reads 34.00 °C, then than sensor is accurate.

Precision is defined as, the ability of a measurement to be consistently reproduced. If on several tests the temperature sensor matches the actual temperature while the actual temperature is held constant, then the temperature sensor is precise and accurate.

Data is said to be reliable if it is reproducible by both yourself and other students. Relevant means that the evidence gives you particular information about the phenomenon you are investigating, not just any data.

3.1.2 Presenting raw data

Raw data is the actual data you measure and may include associated qualitative data (obervations). It is acceptable for you to convert handwritten raw data into word-processed form. The term quantitative data refers to numerical measurements of the variables associated with your Individual Investigation. Associated qualitative data (observations) are considered to be those sensory observations (what you see) that may enhance the interpretation of your results.

Uncertainties are associated with all raw data and an attempt should always be made by you to quantify uncertainties. For example, when there is an uncertainty in a stopwatch measurement because of reaction time, you must estimate the magnitude (size) of the uncertainty.

Within your tables of quantitative data, columns should be clearly annotated with a heading, units and an indication of the uncertainty of measurement. Your uncertainty need not be the same as the manufacturer's stated precision of the measuring device used. If it is not you should state the justification. Significant figures in the data and the uncertainty in your raw data must be consistent. This applies to all measuring devices, for example, digital meters, stopwatches, and so on. The number of significant digits should reflect the precision of the measurement.

There should be no variation in the precision of your raw data for an individual variable. For example, all temperatures may be measured to 1 decimal place (dp) with a particular thermometer. For example, the same number of decimal places should be used. For data derived from processing raw data (for example, means), the level of your precision should be consistent with its calculated uncertainity. The recording of the level of precision would be expected from the point where the you took over the manipulation. For example, you would not be expected to state the level of precision in a solution prepared for you by the school technician.

Recording observations and recognising relevant observations

The accurate and careful recording of **observations** is an important part of the assessment of IB Chemistry coursework. Be aware that simple observations are often the starting point for more detailed quantitative investigations.

Record precise details about the names of any chemicals used, for example, copper(II) sulfate- 5-water, $CuSO_4.5H_2O_{(s)}$. Copper sulfate is ambiguous and may refer to anhydrous copper(I) sulfate, or the various hydrates of copper(II) sulfate.

It is possible to slowly and carefully add solutions to a test tube in such a manner that layers will form. Reaction will only occur at the boundaries giving a banded appearance. Remember to mix your reagents thoroughly before describing your observations. This can be achieved by gently tapping the tube against a finger, gently shaking the tube from side to side or stirring the mixture with a clean glass rod. If immiscible organic solvents are being used, then the tube may need to be stoppered and shaken (though care should be taken to avoid spurting of the contents).

Another type of reaction which may not be directly relevant may be caused by the reaction of two chemicals added to your original sample, for example, the addition of zinc powder and dilute aqueous sulfuric acid will produce hydrogen (and an aqueous solution of zinc sulfate) and this will occur whether or not you have a third chemical–your sample–present.

For gases, indicate whether they fume in air. Describe their colour and intensity (for example, chlorine gas, prepared in a fume cupboard, at high concentrations is pale green), odour (if any – many gases are odourless, for example, hydrogen, oxygen, nitrogen and the oxides of carbon) and effect (if any) on a lighted splint and damp blue and red litmus paper.

Common words used to describe the odour of gases include irritating and choking as well as pungent (ammonia and sulfur dioxide), sweet (dinitrogen monoxide), acidic (hydrogen chloride) and sulfurous or 'rotten eggs' (hydrogen sulfide). To test for the smell of a gas gently waft the gas towards the nose with the hand. Do *not* hold the test tube up to the nose. Some gases, for example, chlorine and, in particular, hydrogen sulfide are highly poisonous.

To bubble a gas through a liquid, for example, carbon dioxide through limewater, use a clean teat pipette. Squeeze the air out of the pipette and draw up a sample of gas from just above the surface of the reaction mixture in the test tube. Now squeeze the teat, expelling the gas through the chosen test solution. Flush the pipette once or twice with this solution.

After recording the odour and colour of a gas (if any) you should conduct, and record the results of, a confirmatory test (*see Figure 301*) that identifies the gas.

Name of gas	Result
Ammonia	Turns pink red litmus blue
Carbon dioxide	Turns limewater (aqueous calcium hydroxide) milky
Sulfur dioxide	A drop of aqueous potassium dichromate(VI) on filter paper is turned from orange to green
Hydrogen	Burns with a squeaky pop
Oxygen	Relights a glowing splint (if dry)
Hydrogen halides	All produce dense white fumes when brought into contact with a drop of aqueous ammonia on a glass rod
Halogens and nitrogen dioxide	Turn blue litmus red and starch-iodide paper blue black. Identify by colour.
Water vapour	Blue anhydrous cobalt(II) chloride paper turns from blue to pink.

Figure 301 Confirmatory tests for common gases

Note that no gas should be described as white. Ammonium chloride formed by the reaction between hydrogen chloride and ammonia gases is best described as a smoke, since it is a suspension of solid ammonium chloride particles in air. A frequent student mistake is to incorrectly use the term 'steam' to describe 'water vapour'. The term 'steam' refers to liquid droplets dispersed in air. The temperature of steam must therefore be below the boiling point of water.

'Water vapour' is the gaseous state of water, and may be formed by evaporation, or by the synthesis of water at room temperature above its boiling point, as in the burning of hydrogen or hydrocarbons. Water vapour is also present in the bubbles formed when water or an aqueous solution are boiled.

There are some additional difficulties that apply to the recording of accurate observations of test tube reactions involving organic chemicals. Organic chemicals are often pure liquids and so, as with solids, the amount of compound present is considerably greater than when solutions are used. Hence, like solids, they should be used sparingly, that is, in small amounts. Many organic liquids, except the lower amines and alcohols, are immiscible or partially immiscible and do not readily dissolve in water. Emulsions may form and these may resemble precipitates. The action of surface tension may cause the droplets to float on the water with the organic liquid (if it denser than water) at the bottom of the tube. Most organic compounds have distinctive odours. You should attempt to group the odours together, for example, fruity (esters), sweet (alcohols), fishy (amines), antiseptic (phenols) etc.

Inexperienced IB Chemistry students often use samples of reagent that are far too large. Solids and pure liquids contain considerably greater amounts of substances than solutions. Therefore, use them sparingly. You will see a small amount dissolve more easily and quickly than a large amount which may be in excess and thus hide the underlying reaction by forming a suspension. Unless otherwise stated, use enough of the solid to fill the hemisphere at the bottom of a test tube.

There are circumstances where you may not be sure if a change has occurred. In these instances use a **control** where a reagent is replaced with distilled water for comparison. If no observable reaction occurs then the chemical was responsible for that change.

If you are adding acid to make an already alkaline solution acidic, check that you have added sufficient acid to neutralise the alkali by using indicator paper. Similarly, check that you have added sufficient alkali if the solution was initially acidic. Ensure the resulting solution is thoroughly mixed before testing its pH. Such solutions should be tested by removing a small drop of the solution with a glass rod and placing on appropriate indicator paper. Do not insert the indicator paper directly into the solution, otherwise contamination will occur.

The IB internal assessment criteria stress that appropriate raw data should be collected. It may not be apparent what observations are relevant and therefore appropriate to record. It is therefore important to record all your observations, no matter how trivial they seem, since some may be important later when you process the raw data and draw a conclusion. The appearance of an organic liquid or solid prepared during an organic synthesis will also allow you to make a qualitative judgement about the purity of your organic sample.

Many students miss important observations with the naked eye even during relatively simple reactions. For example, consider the reaction between a small piece of sodium and water. It is a rare student who (with suitable safety precautions) records that the metal is tarnished (due to the presence of a white oxide layer) and that, when a piece of sodium enters the water, its outer oxide layer is lost and becomes shiny due to the exposure of the underlying silvery metal. The resulting heat is sufficient to melt the sodium and convert it to a molten silvery spherical globule that floats on the surface of the water. If the sodium is confined, the heat may be sufficient to ignite the hydrogen which burns with a golden yellow colour due to gaseous sodium ions.

Examples of recording observations with inorganic reagents

Gas evolution

"*A colourless gas with a pungent (sharp) odour was rapidly evolved. The gas turned moist red litmus paper blue*".

This is better than writing: "*Mixture fizzes off a strong smelling gas. Test with litmus shows gas is alkaline*".

The litmus test is unclear. It is not an observation but a deduction or conclusion. The correct term for the release of bubbles from a liquid surface is effervescence. The relative rate of production of bubbles of gas should also be assessed.

Gases produced by reagents alone are not observations and should not be recorded. For example, aqueous ammonia constantly releases ammonia gas at room temperature and pressure. When you add aqueous ammonia to a solution, you will smell ammonia gas, but this is not a relevant observation.

Colours

It is most important to accurately record the colours of chemicals, for example, indicators and the colours of any light emitted during a practical.

For example, flame tests are used as confirmatory tests for a number of cations (positive ions) or metal ions. Each of these cations when excited thermally emits light of a characteristic colour.

The main areas of confusion are with the three cations that produce reddish flames, namely, calcium, strontium and lithium. The red colours are difficult to describe and, in the case of lithium and strontium, difficult to differentiate. The colours are traditionally described as orange-red (brick red), pink-red (crimson red) and red (carmine red), respectively. Note that the colour you see during a flame test may not be the strongest line in the emission or line spectrum. For example, the strontium flame is pink red, even though the most intense line is in the blue region, because there are many lines in the red region which dominate the emission or line spectrum.

Colour changes

"*The pale blue solution was decolourised*". This is better than writing: "*The pale blue solution went clear*".

What does the word clear mean? Surely the solution was clear when it was pale blue? The opposite of clear is cloudy.

If a solution has no colour, then record the appearance as colourless – it will not be white, since a white 'solution' is never clear, but cloudy, and hence a suspension and not a solution.

It is also important to record all changes that take place during heating. For example, you should record intermediate colour changes of the solid during heating, the change of the solid into the liquid upon heating strongly and the colour of the residue (hot and cold).

Precipitates

"*An off-white precipitate was formed*". This is better than writing "*The solution became dirty white*".

It is not clear if a precipitate has formed. Is it 'dirty', that is, contaminated, or is it undergoing aerial oxidation (for example, iron(II) hydroxide converts to iron(III) hydroxide in the presence of air).

Some precipitates, especially the transition metal hydroxides, are extensively hydrated, and therefore gelatinous (jelly-like).

Some precipitates are photosensitive and undergo partial decomposition. For example, white silver chloride rapidly turns violet, and then black, after precipitation in sunlight:

$2AgCl\ (s) \rightarrow 2Ag\ (s) + Cl_2\ (g)$

Be careful when assessing the colour of a precipitate; a white solid at the bottom of a test tube or boiling tube containing a highly coloured solution often looks coloured.

Always record what you observe, before you write down your (tentative) conclusions or deduction.

For example, you do not see hydrogen, only the bubbles. You observe a colourless and odourless gas, which on testing with a lighted splint burns with a 'squeaky pop'. (Incidentally, the 'pop' involves the formation of water vapour via an explosion (which is exothermic) followed by an implosion as the water vapour condenses into liquid water). These are the observations. The production of hydrogen is an inference.

Negative results should also be recorded, for example, 'No visible reaction' and 'Precipitate did not dissolve'. These can yield useful conclusions or deductions.

Recording Quantitative or Numerical Data

The collection, processing and tabulated displaying of numerical data are important aspects of many IB Chemistry investigations.

Shown below in *Figure 302(a)* is a table of results from a simple investigation into the kinetics of the reaction between 0.15 mol dm^{-3} aqueous sodium thiosulfate and dilute aqueous 1.00 mol dm^{-3} hydrochloric acid.

The student mixed 40.0 cm^3 of sodium thiosulfate with 40.0 cm^3 of acid in a conical flask, on the base of which was drawn a cross, and recorded the time interval (using a data logger connected to a turbidity probe) between mixing the solutions and the mixture becoming sufficiently cloudy that the student could no longer see the cross through the solution. The volumes of the two solutions were measured using a 50 cm^3 measuring cylinder. The measuring cylinder had an error or uncertainty (of ±0.5 cm^3 (at 20 °C).

Volume of 0.15 mol dm^{-3} sodium thiosulfate solution/ cm^3 ±0.5 cm^3	Volume of 1.00 mol dm^{-3} hydrochloric acid ±0.5 cm^3	Volume of distilled water/ cm^3±0.5 cm^3	Time (t) for X to vanish/ s±0.01 s	Rate (1/t)/ s^{-1}
40.0	2.0	0.0	8.00	0.125
30.0	2.0	10.0	11.00	0.091
20.0	2.0	20.0	14.00	0.071
15.0	2.0	25.0	21.00	0.048
10.0	2.0	30.0	32.00	0.031

Figure 302(a) Table of some results from an investigation into the kinetics of the reaction between thiosulfate and hydrogen ions at 25 °C

The effect of sodium thiosulfate concentration on the rate of reaction between sodium thiosulfate and dilute aqueous hydrochloric acid.

These 'rates' are actually pseudo first order rate constants since the concentration of one reactant is considerably greater than the other. It is also perfectly acceptable to have a separate results table to present processed data. Qualitative data concerning colour changes and odours (smells) must also be recorded. Sulfur dioxide has a pungent smell.

Note the following points about *Figure 302* showing a table of results:

- The column headings include the name of the variable and its associated SI units.
- The units are written in the column heading – they should never be written alongside the numerical value.
- Units should not be mixed. For example, all times are in seconds, not minutes and seconds.
- The numbers are presented in decimal form – they should not be presented as fractions.
- A consistent number of **significant figures** has been used for each of the three measurements that comprise the **raw data**, namely, the two volumes and time.
- The **independent variable**(s) of the raw data is/are always recorded in the left hand column of the results table. The volumes of water and sodium thiosulfate are described as independent variables because they were changed by the student. Independent variables are also known as manipulated variables.
- The **dependent variable** of the raw data is always recorded in the right hand side column of the results table. The time is described as a dependent variable since its value depends on the value of the independent variable, namely, the volume of the sodium thiosulfate. The dependent variable is also known as the responding variable.
- The rate values are **processed data** since they are derived from the time values, which are part of the raw data. Processed data are always displayed on the right hand side of the results table or perhaps preferably in a separate results table.
- Processed data are often derived from a mean or average of readings. In this simple kinetic example, each experiment should be performed three times and an average or mean rate calculated. All the individual three times for each of the five concentrations should be recorded. The processing of data may also involve: finding the total, maintaining a running total or calculating differences, logarithms and ratios or percentages.
- The rate values are presented as true numbers, for example, 0.125 rather than .125. It may be preferable to use Scientific notation, for example; 1.25×10^{-1}.
- Raw (unprocessed) data could be separated from processed data to assist your teacher in grading your work according to the Group 4 assessment criteria. However, this is not essential.
- Results tables can be used to generate graphs and both are assessed under the Analysis criterion. They should have a title and should not contain calculations.

Exercise

Identify and correct examples of bad practice in this data table *{Figure 302(b)}* for the cooling of naphthalene.

Time/s	Temperature/°C (±0.5°C)	Temperature/°C
	Trial 1	Trial 2
0	92.0	91.6
30	87.5	88.0
60	83.5	
1 min and 30 s	81	81.00

Figure 302(b) A data table

Uncertainties

All quantitative experiments, for example, titrations and measuring enthalpy changes, involve **uncertainties**.

An error is how much the experimental result obtained differs from the actual value or generally accepted literature value.

It is your responsibility as an IB Chemistry student to identify, quantify (if possible), and, if it is possible, to modify the technique or method and minimise these uncertainties.

The uncertainty of the measurement is reflected by the number of **significant figures** and is expressed as ± (plus or minus) a small amount, for example, a length could be measured as 2.52 cm with a precision of ± 0.02 cm. This means that the actual length will be in the range 2.54 cm to 2.50 cm.

Uncertainties arise from:

- errors due to limitations in the measuring apparatus itself – these, usually quoted by the manufacturer must be considered in your results.
- errors due to limitations in reading the scale on the apparatus–these must be considered, minimised and the direction in which they are likely to affect the result deduced. These errors are usually **random errors**, but may be **systematic errors** if the apparatus is faulty or not used properly.
- errors due to outside factors in the experiment, for example, heat losses, mechanical losses of products during processes such as filtration or transferring of chemicals between glassware–these must be considered and minimised. These errors are usually **systematic errors**.

Types of Errors

There are two types of experimental errors: **systematic errors** or determinate errors and **random errors** or indeterminate errors. (A third type of 'error' known as a human error, mistake or blunder is not an error).

Systematic Errors

Systematic errors result in measured values that are consistently too high or consistently too low. Errors of this type usually are due to identifiable causes and can, in principle, be identified, quantified and, if possible, eliminated.

Types of systematic errors include:

Instrumental

For example, using a poorly calibrated mercury thermometer, that reads 101 °C when immersed in pure boiling water and 1 °C when immersed in ice water at one atmosphere pressure would result in measured values that are consistently too high by a value of 1 °C. Calibration errors may also be present in pH meters and probes, voltmeters, balances, and ammeters. Electronic stopwatches may also have systematic errors due to the presence of almost-flat 'ageing' batteries. A burette may have an internal defect due to the presence of a small fragment of un-melted glass inside the bore. The plungers of gas syringes may stick or leak because of inadequate sealing. (The plunger of a gas syringe should be gently rotated in order to equalise pressures before taking a volume reading). Use of volumetric glassware at temperatures above or below its calibrated temperature (typically 20 °C) will introduce a systematic error. An analogue ammeter might have a bent needle so that it always reads less than it should by a fixed amount.

Observational

A parallax error occurs when the markings of a scale are not physically touching the object, (that is, when there exists a distance between the marking and the object) and the marking is not viewed perpendicularly, as illustrated below in *Figure 303*. This will bring about a relative movement between the object and the markings on the scale when the observer's eye is moved from side to side.

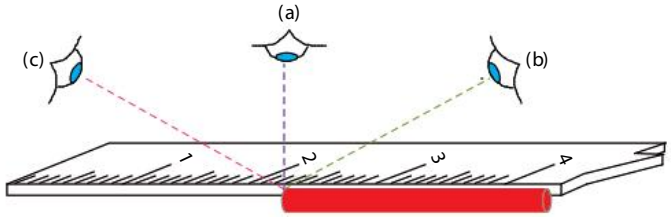

Figure 303 Illustration of the correct and incorrect use of a metre rule

A parallax error exists at positions (b) and (c), but not at position (a).

Reading taken from position (b) = 2.4 cm

Reading taken from position (a) = 2.3 cm

Reading taken from position (c) = 2.2 cm

Parallax errors must also be avoided when using a measuring cylinder, burette or pipette. The volume readings for dilute aqueous solutions or water should always be taken at the bottom of the meniscus: the curved surface of the liquid.

A concave meniscus is formed when the water molecules are strongly attracted to the glass silicate surface, as illustrated in *Figure 304*.

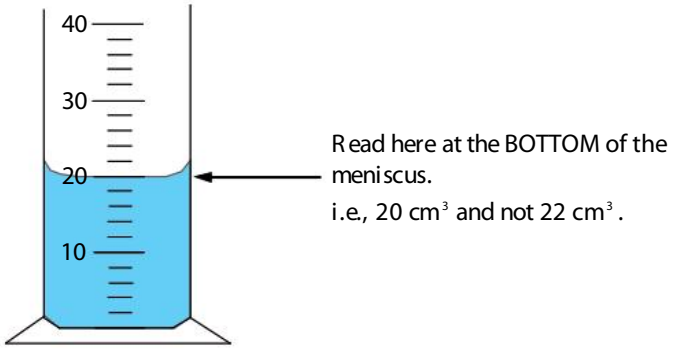

Figure 304 Illustration of the correct use of a measuring cylinder when filled with water or an aqueous solution (concave meniscus)

A convex meniscus is formed when there is little or no glass to liquid attractive force relative to the molecular attraction of the liquid itself, for example when the liquid used is either mercury (for example, in liquid-in-glass thermometers or organic solvents, for example, tetrachloromethane (carbon(IV) chloride), as illustrated below in *Figure 305*.

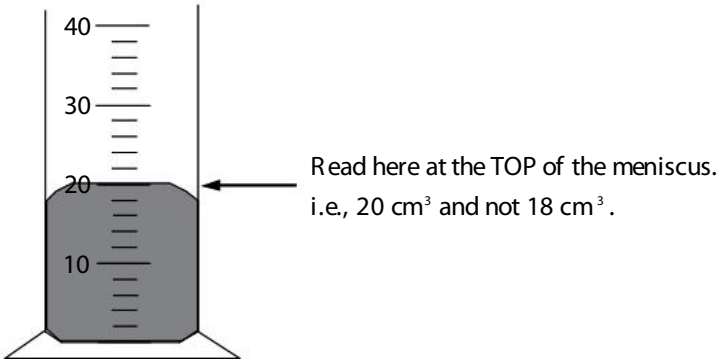

Figure 305 Illustration of the correct use of a measuring cylinder when filled with tetrachloromethane (convex meniscus)

Be aware that systematic errors can sometimes cancel each other out. For example, no overall error would result during a titration if during volume measurements the tops of the meniscuses in the burette were consistently recorded, or if during gravimetric analysis all the weighings were performed on a balance whose readings were consistently too high or too low.

Systematic errors can also be included in your calculation and compensated for, if you are aware of them. For example, if a group of IB Chemistry students were performing the same titration using 25 cm^3 pipettes, but you had accidentally used a 20 cm^3 pipette, your titre volumes would be consistently lower than those of the rest of the group. However, if you have realised this you can apply a correcting factor enabling your results to be compared with those of the other students. Sometimes the very act of recording a measurement can change the value obtained, for example, placing a cold thermometer into a hot liquid or placing an ammeter or voltmeter into an electrical circuit.

Lag time

Some measuring devices require time to reach equilibrium, and taking a measurement before the instrument is stable will result in a measurement that is generally too low. The most common example is taking temperature readings with a thermometer that has not reached thermal equilibrium with its environment.

Systematic errors can also be classified as either proportional errors or constant errors.

Proportional errors either decrease or increase in proportion to the size of the sample. The source of these errors is the presence of interfering contaminants in the sample.

For example, the presence of iron in a sample of brass (an alloy of copper and zinc) interferes with the analysis of copper. The absolute size of the resulting error, in determining the percentage of copper present, is directly proportional to the amount of contaminating iron.

Constant errors are independent of the size of the sample being analysed. They can be minimised by using as large a sample as possible.

For example, consider the recovery of an insoluble solid, such as barium sulfate via filtration. Regardless of the amount of precipitate, a constant percentage of the barium sulfate will be predicted to be adsorbed onto the filter paper – a so-called mechanical loss. However, the filter paper will become 'clogged', that is saturated, so progressively lower percentages will be lost.

Suppose that 0.50 mg of precipitate is lost as a result of being washed with 200 cm^3 of wash liquid. If the precipitate weighs 500 mg, the percentage error due to solubility loss is–(0.50/500) × 100% = -0.1%. Loss of the same quantity from 50 mg of precipitate also results in a percentage error of –1.0%.

The excess of reagent required to bring about a color change during a titration is another example of constant error. This volume, usually small, remains the same regardless of the total volume of reagent required for the titration. Again, in the relative error from this source becomes more serious as the total volume decreases. One way of minimizing the effect of constant error is to use as large a sample as possible.

Detecting systematic errors in an experimental method

There are four methods that can be used to detect systematic errors:

1. Analyse samples of known composition, such as a Standard Reference Material. Your method should reproduce the known answer. Many institutions, for example, for the U.S. National Institute of Standards and Technology or Chemical companies, distribute standard reference materials, such as metals and chemicals that can be used to test the accuracy of analytical procedures used in different laboratories.
2. Analyse blank samples containing none of the substance under analysis to see whether you obtain a non-zero result.
3. Using different analytical methods, for example, titrimetric and gravimetric analysis, to analyse the same substance. If the results do not agree within experimental error, there is systematic error in one (or more) of the methods.
4. Repeated experiments: Identical samples are analysed in the laboratory by other International Baccalaureate Chemistry students using the same or different method. Disagreement beyond the expected random error indicates the presence of one ore more systematic errors.

Theoretical Errors

This type of systematic error occurs due to simplifications or approximations of the chemical or physical model used to describe the chemical system under investigation. For example, if heat losses from a calorimeter are not included in the theory and calculation, then the theoretical and experimental results will consistently disagree. The underlying physical model of this system assumes (mistakenly) that the heat change brought about by the chemical reaction only involves the water and not the surrounding air.

Random Errors

A random error means that a measurement has the same probability of being either equally high or low from one measurement to the next. Random errors are due to chance variations over which you, as an IB Chemistry student, have little or no control. They cannot always be identified. Repetition of an experiment will usually reduce random errors through their tendency to 'cancel out'.

Sources of random errors include:

Observational

For example, errors in the judgment of an IB Chemistry student when reading the scale of a measuring device, for example, measuring cylinder or thermometer, to the smallest division. For example, measuring a volume of 21.2 cm^3 to the nearest 0.2 cm^3 implies a value between 21.1 cm^3 and 21.3 cm^3.

Common random errors in titrations include judging whether the indicator has completely changed colour and whether the bottom of the meniscus is touching the calibration line or 'scratch mark' on the pipette. Other sources of random errors include temperature variations in glassware and temperature and concentration variations in solutions.

Practising good experimental techniques in titrations will help reduce random errors and have a significant effect on the overall accuracy in determining the concentration or percentage purity of a solution or substance. (Colour blindness or other physical handicaps often exacerbate personal random errors).

Environmental

Computerised data collection via the technique of data-logging offers the potential to minimise personal random or systematic errors. However, the electrical circuits themselves suffer from 'noise' which is a source of small random errors in the measurements. The data-logging probe may also lack sensitivity and not respond to very small changes. Experiments that involve measuring volumes of gases will be slightly affected by changes in the surrounding temperature and atmospheric pressure.

Sampling Errors

Errors may arise from unrepresentative samples. For example, suppose you are measuring levels of a particular pollutant in river water. The amount of that particular pollutant may depend on the time of day, the season of the year, etc. So repeated measurements, for example, at 2.00 pm every Thursday may not be representative of the mean or average levels of the pollutant in the river cannot be obtained. Since the sampling technique is so biased a true picture of mean or average levels of the pollutant in the river cannot be obtained. A large population does not of itself ensure greater accuracy.

Precision, Accuracy and Reliability

It is very important to distinguish between the terms: precision, accuracy and consistency.

Accuracy refers to how close an experimental value is to its **true, accepted** or **literature value**. **Precision** refers to the uncertainty of the value that results from the uncertainty values of the measurements from which it is derived. Reliability y refers to how close several experimental measurements of the same quantity are to each other.

If a single IB Chemistry student obtained a series of precise results, the procedure or method is described as **repeatable**. If the same procedure or method is carried out by a number of different IB Chemistry students and precise results are obtained, the procedure is described as **reproducible and the results described as reliable**.

Reliability is thus a measure of the reproducibility of a particular type of measurement. The difference between these two terms is illustrated in *Figure 306* by the results of three different throws of five darts, where the centre of the board, the 'bull's eye', represents the true, accepted or literature value. The size of the dot would represent the precision, and how well they are clustered would represent the reliability.

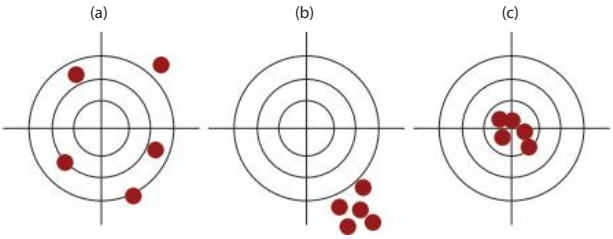

Figure 306 Precision, reliability and accuracy

(a) Neither accurate nor precise and reliable (large random errors are present and the systematic error is negligible in comparison to these). An accurate result can be given if enough values are recorded and the systematic error is negligible.

(b) Precise, reliable but not accurate (small random errors, large systematic error). An accurate result can never be reported.

(c) Both precise, reliable and accurate (small random errors, no systematic error). An accurate result can be obtained from a small set of data readings.

Uncertainties of Measurement

All measuring apparatus, such as thermometers and graduated glassware, e.g., pipettes, have a level of **accuracy** and a level of **precision.**

For example, a micrometer screw gauge from the Physics Department will be more precise and more accurate (assuming no systematic errors) than a small ruler when used to measure the dimensions of a small block of metal.

Precision depends partly on the fineness of the divisions on the scale of the measuring device, and partly on how well the observer can interpolate between divisions on the scale.

If the device is electronic, such as an electronic balance, then the precision depends on the number of decimal places displayed.

For a digital reading, such as from an electronic balance, the last digit is taken as the random uncertainty. For example a balance that measures to 3 decimal places has a random error or uncertainty of ± 0.001 g.

Generally the uncertainty or random error associated with a reading from a scale is reported as half the smallest division or last digit, but further precision may be justified by interpolating between the smallest divisions on the scale. Absolute uncertainties must be included in your raw data under the Analysis criterion.

Sometimes the uncertainty must be predicted at a reasonable level depending of the circumstances. For example, using a pipette (±0.05 cm^3) to measure the volume of a carbonated (fizzy) liquid the uncertainty may increase to ±0.2 cm^3

A temperature change involves two thermometer readings and so, if the thermometer can be read to the ±1^{0}C, it should be known to at least ±2^{0}C, however, measuring a melting point depends on the accuracy of the thermometer used, how quickly the substance was heated and the nature of the apparatus and so could quite reasonably rise to ±3 or 4$^{\circ 0}$C.

Precision of Common Apparatus

Volumetric Glassware

The volume of a liquid is measured using volumetric glassware, which includes measuring/graduated cylinders, volumetric and graduated pipettes, volumetric flasks and burettes. The specific type of glassware used depends on the precision required for the volume measurement.

Volumetric flasks, pipettes, and burettes can measure volumes precisely and are commonly used in titrations. Glassware used as containers, such as beakers and Erlenmeyer/ conical flasks, provide approximate measures and are used when precision is not of paramount importance. Volumetric pipettes deliver specific, fixed volumes and are more precise than graduated pipettes. Volumetric glassware marked "Class A" has twice the precision of the cheaper "Class B" apparatus, sometimes referred to as "economical" or "general use".

A summary of the different types of volumetric glassware and their corresponding precisions and associated uses are shown below in *Figure 307*.

These are general guidelines and you should always examine the glassware you are using and consult the manufacturer's literature, if available. You will also need to indicate the relationship between the instrument limit of error for your measuring instrument and the least count.

Glassware	Precision	Primary use
Graduated Cylinders (Class B)		Delivers approximate volumes
10 cm^3	±0.1 cm^3	
25 cm^3	±0.3 cm^3	
50 cm^3	±0.4 cm^3	
Graduated (Mohr) Pipettes		Delivers more precise volumes
5 cm^3	±0.02 cm^3	
10 cm^3	±0.03 cm^3	
Volumetric Pipette (Class A)		Delivers very precise volumes
5 cm^3	±0.01 cm^3	
10 cm^3	±0.02 cm^3	
25 cm^3	±0.03 cm^3	
Burette		Titrations
50 cm^3 (Class A)	±0.05 cm^3	
50 cm^3 (Class B)	±0.10 cm^3	
Volumetric Flasks (Class A)		Preparation of standard solutions
50 cm^3	±0.05 cm^3	
250 cm^3	±0.12 cm^3	
500 cm^3	±0.20 cm^3	

Figure 307 Precision of Volumetric Glassware

Errors From Apparatus Limitations

The **least count** is the smallest division that is marked on the glassware or scale of the equipment. For example, a 50 cm^3 burette will have a least count of ±0.1 cm^3. The **instrument limit of error** is the precision to which a scale can be read and is always equal to the least count *or* some fraction (e.g., 0.5 or 0.1 etc.) of the least count.

The use of the fraction count as the instrument limit error rather than the least count is justified when the distance between the scale divisions is relatively large. In which case we may, for example, use a specified fraction of the last count as the instrument limit of error, instead of the least count itself.

Hence, although the least count for a 50 cm^3 burette is ±0.1 cm^3, it is possible to distinguish up to 0.05 cm^3 and hence the instrument limit of error could be taken as ±0.025 cm^3. However, in North America, they typically interpolate the scale to 0.02 cm^3 and record the error as ±0.01 cm^3.

This approach to precision (common in North America) may only be justified if the burette being used is of Class A quality and in order to be able to interpolate to the last digit, the perpendicular line of sight must be followed with meticulous care. In addition, the use of a magnifying glass and burette reader would be recommended.

Thermometers

Cheap mercury or alcohol thermometers probably measure to ±1 °C in practice. However, if one considers the scale of a common mercury thermometer (–10 to 110°C graduated to 1 °C), they should, in principle, measure to ±0.5 °C (least count) or ±0.2 °C (instrument limit of error).

Different readings may be obtained using different samples of the same equipment or apparatus. This is particularly true of thermometers. If absolute values of temperature are required rather than differences, it may be necessary to check the readings of the thermometers against each other, or calibrate them in iced water. Cheap thermometers may vary by 0.5 to 1 °C, however, the error when temperature differences are measured, may be reasonably ignored.

When measuring the temperature of a liquid, ensure the bulb of the thermometer is kept under the surface of the liquid. Thermometers are sometimes marked with an immersion depth, or require that the mercury thread be totally immersed under the liquid being tested. In addition, allow sufficient time for the liquid inside the thermometer to reach the temperature of its surroundings.

Mercury thermometers respond more quickly to changes in temperature than alcohol thermometers and tend to give more accurate readings. (Alcohol, like water, does not expand linearly).

The sensitivity of a liquid-in-glass thermometer indicates the ability of the thermometer to measure small changes in temperature. The smaller the capillary bore, the more sensitive the thermometer. This is because there is a larger change in the length of the thread, compared to an identical thermometer with a larger bore, over the same change in temperature. The responsiveness of a thermometer indicates the ability of the thermometer to detect temperature changes quickly. If the thermometer has a thin-walled bulb or contains a small amount of mercury, then a temperature change will cause the thermometer to respond quickly.

Balances

There are many different types of balances with implied precisions of half the final digit varying from ±0.01 g (for a balance that measures to two decimal places) to ±0.00001 g (for a balance that measures to five decimal places).

It is recommended that the origin, justification or derivation of any absolute uncertainty for an experimental measurement be recorded in your Individual Investigation write-up.

Stopwatches

Most electronic stop watches measure to the nearest 0.001 s. Hence the associated error or uncertainty is ±0.001 s

If a stop watch is started and stopped by hand, then a systematic error known as a timing error will occur. This occurs because your hand will take a certain length of time to react, when you are starting or stopping the stop watch. Starting and stopping are not exactly equivalent as the starting can often be anticipated, whilst the stopping cannot.

This error is called the **reaction time** and generally, for the average adult, is in the order of about 0.2 seconds. Thus, a fixed error of 0.2 seconds is introduced when a time interval is measured. Extending the timing period would reduce the percentage error.

Simple Examples of Random and Systematic Errors

Measure and record the mass of an empty measuring cylinder. Fill it about three quarters full of methanol. Record the volume of the methanol in the cylinder. Re-weigh the measuring cylinder and record the mass.

Some possible random errors	Some possible systematic errors
Slight variations in the level of your eye while reading the meniscus in the measuring cylinder. (Assuming that the person's eye is on the same level as the meniscus of the cylinder, i.e., the absence of parallax error). Uncertainty in the reading of the volume in the measuring cylinder.	A poorly calibrated balance will cause all the measured masses to be too high or too low.
Vibrations in the floor or air currents that cause the reading on the balance to fluctuate slightly. Uncertainty in the reading of the mass using the balance.	Methanol evaporates rapidly. During the period of time required to measure its mass, some of the methanol will evaporate. (The occurrence of evaporation could be established by recording the volume of the methanol again after it has been weighed.)

Figure 308 Random and systematic errors in a simple measuring experiment

The random errors (see *Figure 308*), i.e. the uncertainties in the volume and mass readings, can be reduced by taking a number of measurements and then calculating the average or mean. Systematic errors (also *Figure 308*) are caused by the design of the experiments and the limitations of the apparatus used. The systematic errors can be eliminated by calibrating the balance properly and/or by using a cover to prevent evaporation of the methanol. A stoppered volumetric flask would be the ideal type of glassware to perform this simple experiment.

The concepts of random and systematic errors are now applied to a more sophisticated example involving an acid-base titration. An approximately 0.1 mol dm^{-3} solution of aqueous sodium hydroxide is prepared by adding 4.5 g of solid sodium hydroxide to 1000 cm^3 of distilled water.

The precise concentration of the sodium hydroxide solution is determined by titrating it against aliquots of potassium hydrogen phthalate (KHP). (Assume the purity is 100%).

The samples of potassium hydrogen phthalate (KHP) are weighed by difference on a balance.

The reaction between sodium hydroxide and potassium hydrogen phthalate (KHP) is described by the equation:

$NaOH\ (aq) + KHP\ (aq) \rightarrow NaKP\ (aq) + H_2O\ (l)$

The calculation of the concentration of the sodium hydroxide involves the use of the equations given below:

For the solid KHP:

$$\text{Amount of KHP (mol)} = \frac{\text{mass (g)}}{\text{molar mass (g mol}^{-1})} \qquad \text{Equation 1}$$

For the KHP solution:

$$\text{Amount of KHP (mol)} = \text{volume (dm}^3) \times \text{concentration (mol dm}^{-3}) \qquad \text{Equation 2}$$

$$\text{Amount of KHP (mol)} = \text{Amount of NaOH (mol)}$$

$$\text{Amount of NaOH (mol)} = \text{volume (dm}^3) \times \text{concentration (mol dm}^{-3})$$

Combining and rearranging:

Equations 1 and 2

$$\text{Concentration of NaOH (mol dm)}^{-3} = \frac{\text{amount of KHP (mol)}}{\text{volume of NaOH (dm)}^3}$$

$$= \frac{\text{mass of KHP(g)}}{\text{molar mass of KHP (g mol)}^{-1} \times \text{volume NaOH(dm)}^3}$$

Consider the following systematic errors and their effect on the calculated concentration of the sodium hydroxide in comparison to its true concentration:

- The potassium hydrogen phthalate (KHP) was not dried prior to weighing.

  Because of the added water, the measured mass of the potassium hydrogen phthalate (KHP) will be greater than the true mass; therefore the calculated concentration of the sodium hydroxide solution will be greater than the true value. This is because the numerator of the second equation has been increased.

- The balance was not tared or zeroed properly and always gave readings that were 2×10^{-3} g too high.

  The systematic error in the two balanced readings will cancel when weighing by difference, so the measured mass of potassium hydrogen phthalate (KHP) will be the true mass. Therefore the calculated molarity of the sodium hydroxide solution will be equal to the true value.

For example, true masses of KHP: 2.000 g – 1.000 g = 1.000 g and measured masses of KHP: 2.002 g – 1.002 g = 1.000 g

- The sodium hydroxide solution was still warm when titrated against the potassium hydrogen phthalate (KHP), whereas the sodium hydroxide solution is intended for use at 25 °C.

Since solutions expand slightly upon heating, the measured volume of sodium hydroxide solution will be slightly greater than the volume that would have been measured if the solution had been at 25 °C. Therefore, the calculated molarity of the sodium hydroxide will be slightly less than the true value. This is because the denominator of the first equation has been increased.

- When the burette was filled prior to each titration, an air bubble became entrapped in the tip of the burette and was dislodged during the titration by the flowing solution of KHP.

When the bubble becomes dislodged, the level of the meniscus in the burette drops slightly. Hence, the measured volume is slightly higher than the true volume, and hence the calculated molarity of the sodium hydroxide solution will be slightly smaller than the true value. This is because the denominator of the first equation has been increased.

- Using an indicator that changes colour before the equivalence point has been reached.

The end point will be incorrectly identified as a volume that is less than the true volume. Therefore the calculated molarity of the sodium hydroxide solution will be larger than the true value. This is because the denominator of the first equation has been decreased.

- The student did not allow sufficient time for the remaining KHP solution adhering to the burette walls to drain down as the end point was reached.

Because of the KHP solution still adhering to the walls of the burette, the volume of sodium hydroxide that is measured is greater than the true volume. Therefore, the calculated molarity of the sodium hydroxide solution is less than the true value. This is because the denominator of the first equation has been increased.

Type of error	Sources of error	Method of reducing error
Systematic error	• Faulty apparatus or instrument	• Regular maintenance and checking. Correct storage of apparatus or instrument.
Systematic error	• Incorrect calibration of instrument or apparatus (for example, the conditions under which calibration is carried out may be different from those in the school or college laboratory, or the wrong standard was used).	• Re-calibrate correctly, if possible (for example, a pH meter should be calibrated against a fresh buffer, rather than one that has expired or been contaminated with excess acid or alkali).
Systematic error	• Incorrect measuring techniques (for example, generation of a parallax error when consistently reading from a scale incorrectly).	• Use the correct technique when taking readings.
Systematic error	• Problems involving the design of the method for the investigation (for example, no effective control of a particular variable, such as temperature during a kinetics investigation).	• Refine the design of the method for the investigation (for example, the use of a thermostatically controlled water bath instead of an un-insulated glass beaker of water for controlling temperature).
Random error	• Lack of precision on the instrument (for example, using a plastic ruler to measure an object smaller than 1 mm).	• Use an instrument with greater precision or which can detect and measure smaller quantities (for example, using a micrometer screw gauge or vernier calipers).
Random error	• Interpolation between scale divisions (for example, recording readings of a solution level found between two graduations (markings) of a burette.	• Use a magnifying glass.
Random error	• Fluctuations in readings from external factors when measurements are recorded, for example draughts on balance pan causing the digital reading to fluctuate.	• Ensure that environmental conditions are stabilised before recording any measurements.
Random error	• Small sample size	• Increase the sample size
Random error	• The chosen samples are not representative, for example, water samples.	• Repeat measurements for more samples within the same locality and from different localities
Random error	• Variation of consistency by the experimenter in recording measurements. For example, differences in the human reaction time when using the stop watch during an investigation in involving a clock reaction.	• Refine measurement technique, practice recording measurements or use a data-logger in conjunction with an electronic timer/trigger.

Figure 309 A summary of systematic and random errors

Human Errors

Often IB Chemistry students want to classify a human error as an error. However, only systematic and random errors should be included in your error discussion. Human errors, blunders or mistakes, should be noted in your laboratory report, but are not usually included in error discussions.

Common human errors, blunders or mistakes include:

- pouring away all of a liquid product or throwing away all of a solid product before weighing or analysing them.
- performing calculations incorrectly: using incorrect chemical formulas, pressing the wrong buttons on a calculator, calculating units incorrectly etc.
- recording an electronic balance reading etc., incorrectly, for example, recording a mass of 20 g when the true reading was 2.0 g.
- reading a scale backwards.
- not following the correct procedure, for example, using the wrong chemical as a chemical reactant.

These are mistakes that should not have happened and are not usually reported. If they do occur, your results will be invalid and generally cannot be used.

You may have to repeat your experiment(s) or calculation(s), time constraints permitting. There is a 'grey' area between random errors and mistakes. If you are too hasty in performing a measuring procedure, for example, reading a burette then large random errors occur that start to resemble mistakes. Since it is poor judgement the results will have a lot of 'scatter' and it could be asserted that they contain small mistakes.

Non-Errors

No error is introduced since adding distilled water does not alter the amount of alkali (in moles, added from the pipette) in the flask, nor can it change the amount of acid (in moles) added from the burette.

However, cleaning a pipette with distilled water without rinsing it out and then using it in a titration will introduce a small error. The alkali is diluted by the water, so the concentration of alkali added from the pipette is less than assumed in the calculation.

3.1.3 Uncertainties in measurements

Treatment of measurement uncertainties in calculations

During an experiment there will be a number of uncertainties which will have to be considered and processed to give the overall uncertainty. This is known as the **propagation of uncertainties**.

Adding or subtracting measured quantities with associated measurement uncertainties

The maximum absolute uncertainty is the sum of the individual uncertainties.

The rules applied here simplify the computation, but slightly exaggerate the uncertainty at each step. Note that formal mathematical notation is not used.

1. Dealing with uncertainties when one value is being subtracted from another

If the values of two temperatures are 36.3 ±0.1 °C and 56.3 ±0.1 °C, find the difference.

We first subtract the nominal values (56.3 – 36.3) = 20.0 °C.

Then, the absolute uncertainties are 0.1 and 0.1, so we add these, (0.1 + 0.1) = 0.2.

The final answer is 20.0 ± 0.2 °C.

2. Dealing with uncertainties when one value is being added to another

WORKED EXAMPLE

If the values of two temperatures are 36.3 ± 0.1 °C and 56.3 ± 0.3 °C, find the sum.

We first add the nominal values (56.3 + 36.3) = 92.6 °C.

The absolute uncertainties are 0.3 and 0.1, so we add these, 0.3 + 0.1 = 0.4.

The final answer is 92.6 ± 0.4 °C.

The rule for both examples above is to add absolute uncertainties.

Multiplying or dividing measured quantities with associated measurement uncertainties

If uncertainties are to be multiplied or divided then percentage uncertainties have to be used (to take into account that the physical quantities will have different units).

For example, consider the following mass 23.27 ± 0.01 g, the percentage uncertainty is $\frac{0.01}{23.27} \times 100 = 0.4\%$.

The maximum percentage uncertainty is the sum of the percentage uncertainties for each of the individual quantities.

WORKED EXAMPLE

If we want to calculate the power developed during an energy change of 44.01 ± 0.05 J, and the time over which it occurred, namely 2.10 ± 0.05 s, we:

1. take each of the uncertainties.
2. divide it by the given value, and then.
3. multiply by 100 to obtain a percentage.

In this case, for 44.01 ± 0.05 J we have: $\frac{0.05}{44.01} \times 100 = 0.11\,\%$.

For 2.10 ± 0.05 s we have: $\frac{0.05}{2.10} \times 100 = 2.38\,\%$.

The two percentage uncertainties are then added: (0.11% + 2.38%) = 2.49%

So,

$$\frac{(44.01 \pm 0.05)\ \text{J}}{(2.10 \pm 0.05)\ \text{s}} = \frac{44.01}{2.10} \pm 2.49\,\% = 20.96\ \text{J s}^{-1} \pm 2.49\,\%$$

Now, we determine 2.49% of 20.96: $20.96 \times \frac{2.49}{100} = 0.52$

So, our final answer is, 20.96 ± 0.52 J s^{-1} or (20.96 ± 0.52) J s^{-1}.

Note that the relative uncertainty must be converted back into an absolute uncertainty:

i.e., 21 J s^{-1} ± 2.5% = 21 J s^{-1} ± 0.52, but to one significant digit i.e. ± 0.5 since uncertainties are themselves approximate and are not usually given to more than one significant figure.

Therefore

$$\frac{(44.01 \pm 0.05)\ \text{J}}{(2.10 \pm 0.05)\ \text{s}} = 21.0 \pm 0.5\ \text{J s}^{-1}$$

The rule is to convert the absolute uncertainties to percentage uncertainties, then convert them back to an absolute uncertainty after the calculation.

Exercises

Calculate the following percentage uncertainties.

1. 1.00 g on a 2 decimal place balance
2. 10.00 g on a 2 decimal place balance
3. 1.00 g on a 3 decimal place balance
4. 10 cm^3 in a 25 cm^3 measuring cylinder
5. 25 cm^3 in a 25 cm^3 measuring cylinder
6. 25 cm^3 in a 25 cm^3 graduated pipette (Grade B)
7. 25 cm^3 in a 50 cm^3 burette (Grade B)
8. 250 cm^3 in a 250 cm^3 volumetric flask (Grade B)

Worked Examples Of Error Propagation

Worked Example (Thermochemistry)

The heat capacity of a copper can is 50 ± 1 J K^{-1} and in an experiment a temperature rise of 4.0 ± 0.2 °C is obtained.

The uncertainty in the heat capacity is ± 1 J K^{-1}, in **percentage terms** = $\frac{1}{50} \times 100\,\% = 2\%$.

The percentage uncertainty in the temperature reading is $\frac{0.2}{4.0} \times 100\ \% = 5\%$

So, the **maximum percentage uncertainty** is (2% + 5%) = 7%

Now, heat energy released = heat capacity of copper can × temperature rise

= (50 × 4.0) J ± 7% = 200 ± 7% = (200 ± 14) J

(Note, 7% of 200 is 14.)

The answer is best expressed in scientific notation: (2.00 ± 0.14) × 10^2 J = (2.00 ± 0.1) × 10^2 J

Worked example (acid base titrations)

1. Balances

Most chemistry laboratories use digital or electronic balances which typically weigh to 0.01 g. The uncertainty associated with the balance would depend on the mass being measured, but is given by:

$$\%\ \text{error} = \frac{0.01\ \text{g}}{\text{mass g}} \times 100$$

So in an experiment where 10 g of a solid was measured, the percentage uncertainty would be:

$$\%\ \text{error} = \frac{0.01\ \text{g}}{10\ \text{g}} \times 100 = 0.1$$

2. Pipettes

A 25 cm^3 Class A pipette can be read to 0.03 cm^3 and the percentage uncertainty associated with delivering 25.00 cm^3 would be:

$$\%\ \text{error} = \frac{0.03\ \text{cm}^3}{25.00\ \text{cm}^3} \times 100 = 0.12\,\%$$

3. Burettes

A 50 cm^3 burette can be read to 0.05 cm^3. As with the pipette, the uncertainty resulting from the use of this apparatus depends on the amount of solution titrated to reach the end point.

The smaller the volume, the larger the percentage uncertainty. This is why titrations should be planned or designed to obtain the end point when approximately 25 cm^3 of solution have been titrated. In this volume, the percentage uncertainty is given by:

$$\%\ \text{error} = \frac{0.05\ \text{cm}^3}{25.00\ \text{cm}^3} \times 100 = 0.2\,\%$$

4. Volumetric Flask

As with the burette and pipette, the error associated with the use of this type of flask depends on the size of the flask used. A Class A 500 cm^3 volumetric flask is accurate to 0.20 cm^3 and therefore the percentage uncertainty associated with its use would be:

$$\%\ \text{error} = \frac{0.20\ \text{cm}^3}{500\ \text{cm}^3} \times 100 = 0.04\,\%$$

The overall percentage uncertainty, therefore, in using the balance and three pieces of volumetric glassware together is found by adding together the individual percentage uncertainties associated with each piece of apparatus:

Overall percentage uncertainty = (0.1% + 0.12% + 0.2% + 0.04%) = 0.46% (i.e. 0.5%)

Worked example (stoichiometry)

Tin reacts with iodine to give an orange solid of empirical formula SnI_x. In an experiment to find *x*, (3.00 ± 0.01) g of iodine was found to have reacted with (0.70 ± 0.01) g of tin. Deduce the value of *x*. (Molar masses of iodine and tin are 126.9 g mol^{-1} and 118.7 g mol^{-1}).

$$\text{Amount of iodine (mol)} = \frac{\text{mass of iodine (g)}}{\text{molar mass of iodine (g mol}^{-1})} = \frac{(3.00 \pm 0.01)\text{g}}{(126.9\ \text{g mol}^{-1})}$$

$$\text{Amount of tin atoms (mol)} = \frac{\text{mass of tin (g)}}{\text{molar mass of tin (g mol}^{-1})} = \frac{(0.70 \pm 0.01)\text{g}}{(118.7\ \text{g mol}^{-1})}$$

$$x = \frac{3.00\ \text{g}}{126.9\ \text{g mol}^{-1}} \div \frac{0.70\ \text{g}}{118.7\ \text{g mol}^{-1}} = 4.01$$

The molar masses can be regarded as constants so it is necessary only to calculate the uncertainties in the masses of the elements.

$$\text{Percentage error in mass of iodine} = \frac{0.01}{3.00} \times 100 = 0.33\%$$

$$\text{Percentage error in mass of tin} = \frac{0.01}{0.70} \times 100 = 1.43\%$$

The percentage uncertainty in the mass of tin is slightly more than four times that of the iodine; this makes the uncertainty in the weighing of the tin dominant.

Overall percentage uncertainty = (0.33% + 1.43%) = 1.76%

1.76% of 4.00 = 0.0704

Hence $x = 4.00 \pm 0.07$

LOGARITHMS

For logarithmic functions, such as pH, the error is the greatest deviation.

EXAMPLE

A value *y* is calculated from $y = \log_{10} x$

where *x* is measured and found to be 15.43 ± 0.04

The upper limit is 15.47 (i.e., 15.43 + 0.04);

So, we take the logarithm of the upper limit and the nominal value:

$\log_{10}$ 15.47 = 1.1895 and $\log_{10}$ 15.43 = 1.1884

Giving, a deviation of (1.1895 – 1.1884) = 0.0011

Next, the lower limit is 15.39 (i.e., 15.43 – 0.04);

Again, we take the logarithm of the lower limit and the nominal value:

$\log_{10}$ 15.39 = 1.1872 and $\log_{10}$ 15.43 = 1.1884

Giving a deviation of (1.1884 – 1.1872) = 0.0012

The greatest deviation is 0.0012 and therefore $y = 1.1884 \pm 0.0012$ (1.188 ± 0.001).

However, as we can see, the upper and lower limits of deviation are usually very close.

RAISING QUANTITIES TO POWERS

When raising to the *n*th power, multiply the percentage uncertainty by *n*; when extracting the *n*th root, divide the percentage uncertainty by *n*.

For example, w = (4.5 ± 0.2) cm, A = (2.0 ± 0.2) cm^2 and y = (3.0 ± 0.6) cm. Calculate $z = w y^2/\sqrt{A}$.

$$z = \frac{wy^2}{\sqrt{A}} = \frac{4.5\ \text{cm} \times (3.0\ \text{cm})^2}{\sqrt{2.0\ \text{cm}^2}} = 28.638\ \text{cm}^2$$

$$\text{Overall percentage uncertainity} = \frac{0.2}{4.5} \times 100 + 2\frac{0.6}{3.0} \times 100 + 0.5\frac{0.2}{2.0} \times 100 = 49\%$$

The second percentage uncertainty is multiplied by two because the power of y is 2 and the third percentage uncertainty is multiplied by 0.5 since a square root is a power of one half.

49% of 28.638 cm^2 = 14.03 cm^2, which we round to 14 cm^2. Hence z = (29 ±14) cm^2. Because the uncertainty begins with a 1, we keep two significant figures and round the answer to match.

TRIGNOMETRIC FUNCTIONS (Extension Material)

The IB Chemistry syllabus does not require a knowledge or use of trigonometry. However, it might be required in an experimental situation, for example, an investigation involving the use of Bragg's law or polarimetery. However, these are topics outside the current IB Chemistry syllabus, but your own research and review may have lead you to utilise such concepts in your Individual Investigation.

The error or uncertainty in a trignometric function such as sin(x) can be estimated as being the difference between the largest possible value and the average value.

Hence if Δ represents the error then $\Delta(\sin x) = \sin(x + \Delta x) - \sin(x)$.

For example, $A = x \cos(\theta)$ for $x = 2.0 \pm 0.2$ cm, $\theta = 53 \pm 2°$.

A = (2.0 cm) cos 53 ° = 1.204 cm

To obtain the largest possible value of A make x larger, (x + Δx) = (2.0 + 0.2) = 2.2 cm and θ smaller, (θ–Δθ) = (53–2) = 51°.

The largest value of A, namely, (A + ΔA), equals (2.2 cm) cos 51° = 1.385 cm. The difference between these numbers is 0.181 cm which is rounded to 0.18 cm, hence A should be reported as 1.20 ± 0.18 cm.

Calculating Percentage Error

Chemists check the accuracy of their measurements by comparing their results with values that are well established in the chemical literature and are considered to be 'accepted values'. For IB Chemistry students the 'chemical literature' usually refers to a text book or the IB Chemistry Data Booklet. It is most important that the results from all your experiments are compared with the literature values, even if the results are as expected.

To report the percentage error in your result, take the absolute value of the difference between your value and the accepted value, divide this difference by the accepted value, and then multiply by 100.

Taking *x* to be your measured value and *y* to be the accepted value:

$$\text{Percentage error} = \left|\frac{x-y}{y}\right| \times 100\ \%$$

Example

The experimentally determined enthalpy change for a reaction is 50.0 kJ mol^{-1} and the accepted, true, or literature value is 75.0 kJ mol^{-1}.

Percentage error =

$$\left|\frac{(75.0 - 50.0)}{75.0}\right| \times 100\,\% = 33.3\,\%$$

The percentage error is expressed to the same number of significant figures as the two enthalpy values, i.e., three.

The **absolute error** is the difference between the experimental value and the literature value, i.e., absolute error = (75 – 50) = 25 kJ mol^{-1}.

Error Analysis

Error analysis is an important part of an IB Chemistry practical program but the lengthy process of error analysis should not overshadow the investigation or detract from the conclusions of the investigation.

The basic principle of error analysis is to compare **percentage error** with **percentage uncertainty**. Two worked examples are provided below.

An example of error analysis for a thermochemistry or calorimetry experiment involving neutralisation is shown below.

Example

The temperatures before and after the enthalpy change were as follows:

$T_1 = 21.2 \pm 0.2$ °C

$T_2 = 23.2 \pm 0.2$ °C

$\Delta T = T_2 - T_1 = 2.0 \pm .4$ °C

Note: recall the rule that, during addition and subtraction, the absolute

uncertainties are added together.

So, the percentage uncertainty = $\frac{0.4}{2.0} \times 100\,\% = 20\,\%$.

Now, $Q = m \times c \times \Delta T$,

where Q is the quantity of heat released, m is the mass of water,

c is the specific heat capacity of water and ΔT is the rise in temperature.

So that, $Q = 200\ \text{g} \times 4.18\,(\text{J g}^{-1}\,^{\circ}\text{C}^{-1}) \times 2.0\,^{\circ}\text{C} = 1672\ \text{J}$.

If this temperature rise is due to the reaction of 0.0500 mol of aqueous hydrochloric acid added to 0.0500 mol of aqueous sodium hydroxide then:

$$\Delta H = \frac{-1672\ \text{J}}{0.0500\ \text{mol}} = -33440\ \text{J mol}^{-1} = -33.4\ \text{kJ mol}^{-1}$$

If the accepted or literature value for this reaction is – 56.2 kJ mol^{-1}, the percentage

difference is:

$$\left|\frac{(56.2 - 33.4)}{56.2}\right| \times 100 = 40.6\,\%$$

Assuming the uncertainties in the mass of water (m), the specific heat capacity of water (c) and the amounts of acid and base are very small compared with the large uncertainty of the temperature, then the percentage error of 40.6% is greater than the percentage uncertainty due to random errors, of about, 20%.

This discrepancy indicates that random errors alone cannot account for the difference between the experimentally determined value and the literature value. Systematic errors must account for this difference. IB Chemistry students should always try to identify these systematic errors, decide whether these are consistent with the direction of the percentage error and suggest improved methods for performing the experiment. Error analysis is an important part of the IB Chemistry practical program and its assessment.

For example, a highly conducting open metallic container may have been used as the calorimeter thereby giving rise to significant heat loss from the system, which would have given a lower enthalpy of reaction as was observed. The systematic errors could therefore be reduced by insulating the calorimeter and providing it with a lid.

The second worked example involves the determination of the gas constant, R, using the Ideal Gas Equation ($PV = nRT$), where P represents the pressure, V represents the volume, n represents the amount of gas (moles) and T represents the absolute or thermodynamic temperature.

The data below include percentage uncertainties in each of the pressure, volume, amount and absolute temperature measurements where nitrogen gas is produced and collected by displacement of water.

(Note: there are several assumptions regarding this experimental approach, namely, that the nitrogen gas does not dissolve or react with water to any appreciable extent, that the apparatus used is air tight and that nitrogen is behaving ideally under these experimental conditions).

$P(N_2) = 98.1 \pm 0.23\%$ kPa; $V(N_2) = 0.363 \pm 0.55\%$ dm^3; $n(N_2) = 0.0147 \pm 1.05\%$ mol and $T(N_2) = 298.8 \pm 0.07\%$ K.

Example

The total uncertainty = (0.23% + 0.55% + 1.05% + 0.07%) =1.9%

$$PV = nRT \Leftrightarrow R = \frac{PV}{nT} = \frac{98.1\ \text{kPa} \times 0.363\ \text{dm}^3}{0.0147\ \text{mol} \times 298.8\ \text{K}}$$

$$= 8.11\ \text{kPa dm}^{-3}\ \text{mol}^{-1}\ \text{K}^{-1} \text{ or } 8.11\ \text{J mol}^{-1}\ \text{K}^{-1}.$$

The percentage difference between the experimentally determined value and the literature value is given by:

$$\left|\frac{(8.31 - 8.11)}{8.31}\right| \times 100 = 2.41\,\%$$

As with the previous example involving calorimetry, the percentage difference is greater than the percentage uncertainty and as a consequence random errors alone cannot account for the difference. There must be systematic errors inherent to the investigation or the apparatus.

The most likely explanation is the loss of nitrogen from the apparatus (hence a decrease in the volume, V) and the failure to 'correct' for the vapour pressure of water vapour (hence a decrease in the pressure, P). Either would result in a value of the ideal gas constant, R, which is smaller than the literature value, as is observed.

UNCERTAINTIES IN AN AVERAGE OR MEAN (Extension Material)

As we have seen previously the accuracy of measurements can be improved by taking additional readings and averaging the results.

For example, suppose that a metal block was measured (with vernier calipers with no zero error) and the following measurements were obtained:

1.25 cm, 1.24 cm, 1.22 cm, 1.22 cm, 1.26 cm and 1.24 mm

The average is thus 1.24 cm and the reading which differs most widely from the mean, namely, 1.26 cm, does so by 0.02 mm.

The percentage error in the mean can be calculated:

$\frac{0.02}{1.24} \times 100 = 1.6$ % or 2%, when expressed as one significant figure.

This is only of several possible mathematical approaches. A more sophisticated statistical approach involving standard deviation, can also be employed but is only applicable if the number of repeated measurements is large and follows a Gaussian or normal distribution.

Miscellaneous advice about errors or uncertainties

- Do not worry about the errors in the errors.

Errors, by their very nature, cannot be precisely quantified. Hence, a length reported as (2.733 ± 0.313) m is excessively precise and should probably be reported as (2.7 ± 0.3) m. So as a general rule:

Errors should be usually quoted to one significant figure; two significant figures are sometimes justified, especially if the figure in the measurement is a one.

- Neglecting small errors

When calculating errors in sums and difference, ignore any errors that are less than ⅓ of the largest error, and when calculating errors in products and ratios, ignore any percentage error that is less than ⅓ of the largest error.

Concentrate on reducing the dominant errors

- The largest errors will dominate the error in the final result, and small errors can often be neglected. It is therefore important that when carrying out an investigation that not to waste time reducing small errors when much larger errors are also present.

Try and determine what the dominating errors in an investigation are, and then concentrate on reducing them.

- Take care when differences and powers are involved, since they can give rise to overall errors which are much larger than the errors in the individual

3.2 Data Processing

Guiding questions:

- *Has the student selected an appropriate method for analyzing the data?*
- *How successfully has the student analysed the data?*

Introduction to data processing

Data processing involves, for example, combining and manipulating raw data to determine the value of a physical quantity (such as adding, subtracting, squaring, dividing and performing logarithms or anti-logarithms and taking the average or other statistic of several measurements and transforming data into a form suitable for graphical representation.

It might be that the data is already in a form suitable for graphical presentation, for example, light absorbance readings plotted against readings of a coloured substance at different concentrations. If the raw data is represented in this way and a best-fit line graph is drawn and the gradient determined, then the raw data has been processed. Plotting raw data (without a graph line) does not constitute processing data. The recording and processing of data may be shown in one table provided they are clearly distinguishable.

The study of Kinetics is an important part of the IB Chemistry Programme and lends itself well to practical work for the Individual Investigation. However, it is a difficult topic, partly because it has an empirical side and a theoretical side which interlink. Establishing rate equations is an important part of investigative work in kinetics. The section below provides detailed guidance on how experimental data should be processed and analysed.

Establishing a Rate Expression

Initial rates

One method for determining the rate expression is to experimentally measure how the concentration of a reactant or product varies with time and then construct characteristic kinetics plots. Another approach to determining the rate expression is to use the method of initial rates.

The method of initial rates involves measuring the rate of reaction at very short times before any significant changes in concentration occur. Many reactions have a rate expression of the following form:

rate = k $[A]^a$ $[B]^b$ etc.

The initial concentrations of the reactants A and B are known; therefore, if the initial reaction rate is measured, the only unknowns in the rate law are the rate constant, k, and the exponents a and b (the individual orders). An IB student would typically measure the initial rate for several different sets of concentrations and then compare the initial rates.

Consider the following set of data:

TRIAL	RATE (mol dm^{-3} sec^{-1})	INITIAL CONCENTRATION OF A (mol dm^{-3})	INITIAL CONCENTRATION OF B (mol dm^{-3})
1	2.73	0.100	0.100
2	6.14	0.150	0.100
3	2.71	0.100	0.200

If simple multiples are chosen for the concentrations and only one concentration is varied at a time, an IB student can determine a and b by inspection. The IB student can also employ the following algebraic technique for determining the exponents.

First, write the ratio of the rate laws for two trials.

$$\frac{rate_1}{rate_2} = \frac{k[A]_1^a[B]_1^b}{k[A]_2^a[B]_2^b}$$

Next, substitute the numerical values into the equation:

$$\frac{2.73 \text{ mol dm}^{-3} \text{ s}^{-1}}{6.14 \text{ mol dm}^{-3} \text{ s}^{-1}} = \frac{\text{k } (0.100 \text{ mol dm}^{-3})^a \ (0.100 \text{ mol dm}^{-3})^b}{\text{k } (0.150 \text{ mol dm}^{-3})^a \ (0.100 \text{ mol dm}^{-3})^b}$$

Notice that the units for each quantity and the rate constant can be removed, and in this case the exponent *b* is removed when the concentrations of reactant B divide. The equation simplifies to:

$$\frac{2.73}{6.14} = \frac{0.100^a}{0.150^a}; \quad 0.4446 = 0.6667^a$$

To convert *a* from an exponent into a coefficient, take the logarithm of both sides of the equation.

$\ln[0.4446] = \ln[0.6667a]$ $-0.8106 = -0.4054a$

The value of *a* may now be readily determined:

$a = \frac{-0.8106}{-0.4054} = 1.9995$, hence the reaction is second order with respect to A = 0.4054

In most experimental situations the exponents will be 0, 1 or 2. A similar approach can be used to determine the value of *b*, which is obviously zero order. Once the exponents are known, the rate constant can be calculated. However, since the data suffers from experimental error, it is best to calculate the rate constant for each trial and use the average value.

Isolation Method

Another approach to establishing rate expressions is the isolation method. In this method the concentration of one reactant is made considerably smaller than the concentrations of the other reactant(s).

(*Typically a 20 fold stoichiometric excess is effectively required to 'isolate' the effects of a single reactant, but a 50-fold or 100-fold, as in the example below, stoichiometric excess is preferable.*)

Under this condition, all reactant concentrations except one are essentially constant, and the simple zero-, first-, and second-order kinetic plots can be used to interpret the concentration-time data. The shapes of typical concentration-time graphs are shown below in *Figure 310*. A first order reaction has a constant half life.

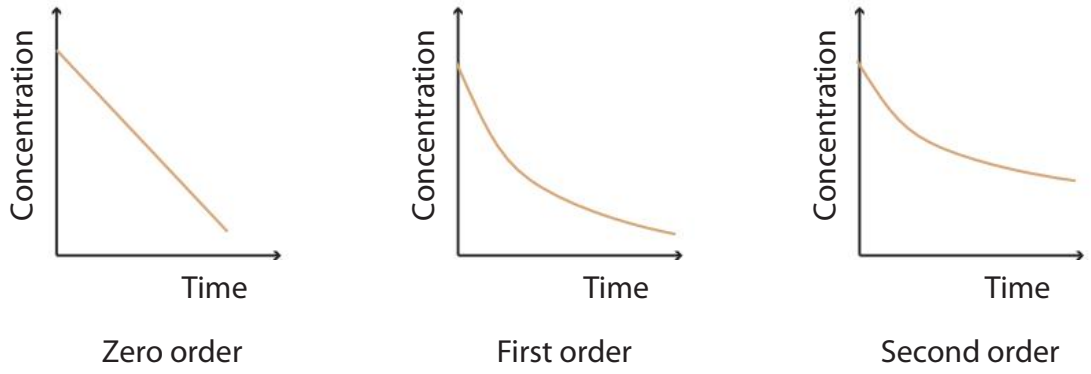

Figure 310 Reactant concentration-time graphs

To observe how this approach works consider the following substitution reaction where bromomethane is hydrolysed to methanol:

$CH_3Br\ (aq) + OH^-\ (aq) \rightarrow CH_3OH\ (aq) + Br^-\ (aq)$

The rate expression for this substitution reaction is first-order with respect to bromomethane and first-order with respect to hydroxide ion. This reaction proceeds via an S_N2 mechanism where the hydroxide ion and the bromomethane molecule are both involved in the rate determining step.

Hence it is second-order overall.

rate = $k\ [CH_3Br\ (aq)]\ [OH^-\ (aq)]$

If reaction were performed starting with 0.100 mol dm^{-3} aqueous sodium hydroxide and 0.001 mol dm^{-3} CH_3Br. When the reaction is finished, the solution will contain 0.099 mol dm^{-3} sodium hydroxide and no bromomethane (limiting reagent). Notice that the concentration of hydroxide ion is virtually unchanged. The value of the hydroxide ion concentration can therefore be treated as a constant, and the rate expression simplifies to:

rate = $k_{observed}\ [CH_3Br\ (aq)]$

which is a simple first-order rate expression. The observed rate constant, $k_{observed}$, is a pseudo-first-order rate constant. The reaction is a pseudo-first-order reaction, because it behaves as if it were first-order. The difference is that $k_{observed}$ is not constant; it varies with the initial concentration of hydroxide ions.

$k_{observed} = k\ [OH^-\ (aq)]$

In practice, an IB student would perform a series of experiments in which the hydroxide varies but was always much larger than the initial concentration of bromomethane. For each experiment, $k_{observed}$ would be determined, and the student would then prepare a plot of $k_{observed}$ versus $[OH^-]$ for a minimum of five pairs of data values. The graph will be linear with a gradient of the line of best fit equivalent to the rate constant, k.

If the student did not know the reaction was first-order with respect to hydroxide ion, the exponent for the hydroxide ion concentration could also be determined from the experimental data. The observed rate constant would be

$k_{observed} = k\ [OH^-(aq)]^x$

Taking the natural logarithm of both sides of this equation leads to

$\ln k_{observed} = \ln k + x \ln [OH^-\ (aq)]$

A plot of $\ln k_{observed}$ versus $\ln [OH^-]$ produces a straight line with a gradient equal to b and intercept equal to $\ln k$.

Hence a student can simultaneously determine b and k, and the method works for any value of x.

Note the following points:

- Although the reaction is first order with respect to bromomethane the rate constant cannot be calculated from the expression: $k = \frac{\ln 2}{t_{1/2}}$. This is because the expression is only valid for a first order reaction. The reaction is second order.
- If equal concentrations of bromomethane and hydroxide ions were used then a very poorly designed experiment has been implemented. The rate will decrease based on the order of both bromomethane and hydroxide ions. It will then be difficult to establish the order by plotting concentration of bromomethane versus time since the decrease is affected by both bromomethane and hydroxide ions.

Below is an example (with inserted comments in italics) of how raw data is processed to obtain the enthalpy change of the replacement reaction between copper(II) ions and zinc metal.

$Zn\ (s) + Cu^{2+}\ (aq) \rightarrow Zn^{2+}\ (aq) + Cu\ (s)$

0.25 mol dm^{-3} copper(II) sulfate solution (prepared by school technician); 50 ± 1 cm^3

Mass of zinc powder = 0.99 ± 0.02 g

Maximum final temperature = 33.4 ± 0.5 °C; initial temperature = 24.0 ± 0.5 °C

Temperature rise = 33.4 °C–24.0 °C = 9.4 ± 1 °C = 9 ± 1 °C

(Add absolute uncertainties when subtracting measurements; adjust the answer to match precision of the uncertainty)

Amount of copper(II) ions = $\frac{50}{1000} \times 0.25 = 0.0125$ mol (1 s.f.)

Absolute uncertainty = $\left(\frac{1}{50}\right) \times 0.0125 = 2.5 \times 10^{-4} = 0.0003$ mol (1 s.f.).

(It is very helpful to your IB Chemistry Teacher and the moderator appointed by the IBO to show your working with uncertainties or errors and demonstrate that you have applied the significant figure rules. One approach is to divide the page into two: calculations on the left; error propagation on the right).

(The uncertainty is expressed to 1 s.f. since 1 has 1 s.f.)

Amount of zinc atoms = $\frac{0.99}{65.37} = 0.0151$ (3 s.f.)

Absolute uncertainty = $\left(\frac{0.02}{0.99}\right) \times 0.0151 = 3.05 \times 10^{-4} = 0.0003$ mol (1 s.f.)

(The uncertainty is expressed to 1 s.f. since 0.02 has 1 s.f.)

Copper(II) ions are the limiting reagent, hence amount = 0.0125 ± 0.0003 mol

Assuming that 4.2 Joules of heat is required is required to raise the temperature of a dilute aqueous solution by 1 °C and that the density of the solution is 1.00 g cm^{-3}.

Specific heat capacity = (50 cm^3 × 1.00 g cm^{-3}) × (4.2 J g^{-1} $°C^{-1}$) × 9 °C = 1890 J

Absolute uncertainty = $\left(\frac{1}{50}\right) + \left(\frac{1}{9}\right) \times (1890) = 247.8$ J = 248 J (1 s.f.)

Hence, heat energy produced = 1890 ± 248 J

Enthalpy change of replacement = $-\left(\frac{1890}{0.0125}\right) = 151\,200$ J mol^{-1} = 151 kJ mol^{-1} (3 s.f.)

(The *uncertainty is expressed to 3 s.f. since 0.0125 has 3 s.f.,)*

Absolute uncertainty = $\left(\frac{300}{1890}\right) + \left(\frac{0.0003}{0.0125}\right) \times (151200) = 27\,630$ J mol^{-1}

Hence, enthalpy change of replacement = -151 ± 28 kJ mol^{-1}

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Common mistakes made during numerical calculations include:

- Incorrect calculations for the molar masses of hydrated salts, for example, $5H_2O$ = 10 +16 g mol^{-1}, instead of 10 + 80 = 90 g mol^{-1}
- Assuming that 22.7 dm^3 represents the volume of one gram instead of the volume of one mole of gas (at S.T.P.)
- Giving only the bare calculation without mentioning the laws and principles involved
- Introducing *x* without stating what it represents
- Forgetting to attach units to the numbers given as a result
- Leaving the result as a fraction
- Stating the result with the wrong number of significant figures
- Not checking that your answer appears reasonable
- Not expressing the final answer with an absolute uncertainty
- Not showing all your working: numerical calculations and error propagation

3.2.1 Significant figures in calculations

Significant Figures: Concept And Definition

Imagine that you have prepared a solution of chemical X and that you need to determine its concentration by titration against a primary standard.

Imagine that you have weighed out 14.87 g of chemical X. Your sample may contain as little as 14.865 g or as much as 14.874 g on a balance reading to 0.001 g, since the last digit is 'rounded up' or 'rounded down' by the instrument. Therefore, any mass between 14.874 g and 14.865 g would register as 14.87 g on a balance reading to 0.01 g. 14.864 g would have registered as 14.86 g and 14.875 g would have registered as 14.88 g (see *Figure 311*).

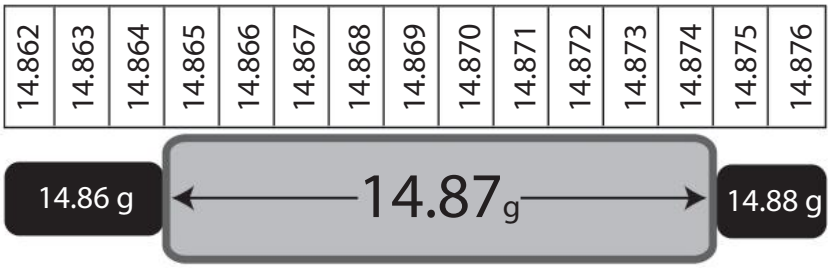


Figure 311 A balance reading of 14.87 g

The balance reading of 14.87 g contains four figures and these are all described as **significant figures**. You can think of significant figures as being certain or reliable; we do not know whether (on a balance with this precision) you really have 14.870 g or 14.871, or even 14.874 g. In other words, we do not know what the fifth value is in a mass value.

Generally, all measured quantities in Chemistry are generally reported so that the last digit is uncertain. This mass could be reported as 14.87 ± 0.005 g. The upper and lower limits are 14.87 g + 0.005 g, that is, 14.875 g and 14.87 g – 0.005 g, that is, 14.865 g.

The concept of a significant figure can also be illustrated with a scale. For example, consider the reading of a thermometer scale, part of which is shown in *Figure 312*, some International Baccalaureate Chemistry students may record the temperature as 28.2 °C and, others may, in equal numbers, record it as 28.1 °C and 28.3 °C.

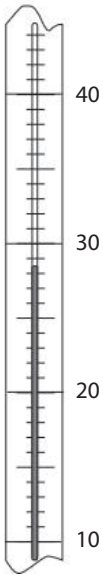


Figure 312 Part of a thermometer scale (magnified)

There is no doubt that the temperature is between twenty one and twenty two degrees Celsius, but there is uncertainty in the final figure. This temperature should therefore be reported as 28.2 ± 0.1 °C. The upper and lower limits are 28.2 + 0.1 °C , that is, 28.3°C and 28.2 – 0.1°C , that is, 28.1 °C. The temperature value is thus reported to three significant figures.

These two examples both show that significant figures must be considered whenever a chemical or physical property is measured and its value recorded. Furthermore, it is important to consider the use of significant figures when calculations are performed using electronic calculators, which may display up to ten digits on their display. You are very rarely in justified in using all of them.

Counting The Number Of Significant Figures

The number of **significant figures** in a numerical result is an indication of the accepted error in a number. In counting the number of significant figures the problem is the digit zero (0). There are five rules used in counting the number of significant figures in a number:

1. All non-zero digits are significant,

e.g., 12.3 has three significant figures and 549 has three significant figures.

2. Zeros between non-zero digits are significant,

e.g, 1.03 has three significant figures and 4023 has four significant figures.

3. Zeros at the end of a number are significant,

For numbers with decimal points, zeros to the right of a non zero digit are significant. E.g., 2.00 has three significant figures, but 0.050 has two (the 5 & 0 in the second and third decimal places).

4. Zeros to the left of the first non zero digit are not significant,

e.g., 0.84 has two significant figures: eight and four. The zero is termed a *placeholder*, meaning the zero is not part of the measurement, i.e., it is not significant.

5. Zeros at the end of a number without a decimal point are ambiguous,

e.g., 80 may have two significant figures or it may have one – the eight – with the zero being a place holder. Only the person who carried out the measurement would know. The ambiguity can be removed by reporting such numbers in scientific or standard notation. For example, writing 80 as 8×10^1 means that only one significant figure is present (a ±5 error), while writing it as 8.0×101 means that two significant figures are present (a ±0.5 error).

6. Many physical constants, have a very large number of digits,

e.g., the speed of light in a vacuum, *c* (299 792 458 m s^{-1}).

(In theory, infinite, but in practice limited by the precision of the measuring device).

7. Mathematical constants,

e.g., a number such as pi (π) has an infinite number of digits

8. Logarithms can only retain in their mantissa the same number of significant figures as there are in the number whose logarithm you are taking.

Rounding Off

Sometimes it is necessary to round off, to give the correct number of significant figures.

1. A digit of 5 or larger rounds up.
2. A digit smaller than 5 rounds down.

For example, rounding 13.654 to three significant figures gives 13.7 (the 4 is ignored, the 5 rounds up).

For example, rounding 13.246 to three significant figures gives 13.2 (the 6 is ignored, the 4 rounds down).

Worked Example

In an experiment to measure the enthalpy change of reaction the following measurements were made:

Mass of water = 58.000 ± 0.0005 g

Temperature change of water = 12.5 ± 0.05 °C

Heat released = mass of water × specific heat capacity of water × change in temperature

= 58.000 g × 4.184 J g^{-1} $°C^{-1}$ × 12.5 °C

= 3033.4 J

The temperature change was the **least** precise measurement (three significant figures) so the result cannot be expressed as having more than three significant figures.

Therefore the answer is 3030 J or, better still, 3.03×10^3 J and **not** 3033.4 J.

It is unacceptable to report values with more significant figures than indicated by the associated uncertainty. For example, in 8.37 ± 0.2 cm the seven has no meaning and the length should be reported as 8.4 ± 0.2 cm.

Exercises

Underline the number of significant figures in the following numbers.

(a) 0.0420 cm

(b) .320 J

(c) 10 kg

(d) 0.020 cm^3

(e) 2403 dm^3

(f) 80.5300 m

(g) 2.4×10^3 kg

Significant Figures In Arithmetic

In this section we address the issue of how many digits you should retain in your answer after you have performed arithmetic operations with your experimental data.

'Rounding' of your answer should only be carried out on the final answer (not the intermediate results) to avoid so-called round-off errors.

Addition and Subtraction

If the numbers that are to be added or subtracted have the same number of decimal places, the answer should be expressed to the same number of decimal places as in each of the individual numbers:

$$\begin{array}{r} 1.361 \times 10^{-4} \\ +\ 3.112 \times 10^{-4} \\ \hline 4.473 \times 10^{-4} \end{array}$$

In the example above all the numbers are expressed to three decimal places.

The number of significant figures in the answer may be greater than or less than in the original data.

$$\begin{array}{r} 5.346 \\ +6.728 \\ \hline 12.074 \end{array}$$

The answer has five significant figures but the data has four significant figures.

$$\begin{array}{r} 7.27 \times 10^{14} \\ -6.68 \times 10^{14} \\ \hline 0.57 \times 10^{14} \end{array}$$

$= 0.59$

The answer has two significant figures but the data has three significant figures.

If the numbers being added do not have the same number of significant figures, then you are limited by the least certain one.

$$\begin{array}{r} 18.998\ 404 \\ +18.998\ 404 \\ +83.80 \\ \hline 121.796\ 808 \end{array}$$

The number 121.796808 should be rounded to 121.80 as the final answer. Note that the answer is expressed to two decimal places since the third datum, the least precise, is expressed only to two decimal places.

When 'rounding-off' your answer look at all the digits displayed by your calculator beyond the last place desired.

In this example the digits 6 808 lie beyond the last significant decimal place. Because this number is more than half way to the next higher digit, we round the number 9 up to 10 (that is, we round up to 121.80 instead of down to 121.79).

(In the special case where the number is exactly halfway, round to the nearest even digit. For example, 43.550 00 is rounded to 43.6 if the number is to be expressed to three significant figures). The rationale for rounding an even digit is to avoid systematically increasing or decreasing results through successive round-off errors. Half the round-offs will be up and half down.

When adding or subtracting numbers expressed in scientific or standard notation, all numbers should be first expressed with the same exponent:

$$\begin{array}{l} 1.631 \times 10^5 \\ +4.107 \times 10^3 \\ \underline{+0.985 \times 10^6} \end{array}$$

$\Rightarrow$

$$\begin{array}{l} \quad 1.631 \times 10^5 \\ +\ 0.041\ 07 \times 10^5 \\ \quad +\ 9.85 \times 10^5 \\ \hline \quad 11.51 \times 10^5 \end{array}$$

$= 11.52$

The sum $11.522\ 07 \times 10^5$ is rounded to 11.52×10^5 because the number 9.85×10^5 limits the answer to two decimal places when all the numbers are expressed as multiples of 10^5.

Multiplication and Division

In multiplication and division you are limited to the number of digits contained in the number with the fewest significant figures:

$$\begin{array}{l} 3.26 \times 10^{-5} \\ \underline{\times\ 1.78} \\ 5.80 \times 10^{-5} \end{array}$$

Both the answer and data each have three significant figures.

$$\begin{array}{l} 34.60 \\ \underline{\div 2.462\ 87} \\ 14.05 \end{array}$$

The answer is expressed to four significant figures since the least precise number (34.60) has four significant figures.

Logarithms and Antilogarithms

A logarithm may be considered to be composed of a character and a mantissa. The character is the integer part and the mantissa is the decimal part:

$\log_{10} 339 \quad = \quad 2.530\ 199$ etc.

Character **Mantissa**

The number 339 is written as 3.39×10^2 in Scientific or standard notation. The number of digits in the mantissa of $\log_{10} 339$ should equal the number of significant figures in 339. The logarithm (to the base 10) of 339 is therefore 2.530.

This 'rule' should be applied to the conversion of hydrogen ion molarities into pH values.

$[H^+ (aq)] = 3.39 \times 10^{-5}$ mol dm^{-3}; $\log_{10} 3.39 \times 10^{-5} = -4.470$; pH = 4.470

(However, from an experimental viewpoint pH values should only be quoted to two decimal places).

In converting a logarithm to its antilogarithm, the number of significant figures in the antilogarithm should equal the number of digits in the mantissa. This 'rule' should be applied to the conversion of pH values into hydrogen ion molarities.

For example: pH = 4.37;

$[H^+ (aq)]$ $= 2.3 \times 10^{-4}$ mol dm^{-3}

(Antilog 4.37 $= 2.3 \times 10^4$)

	Rule	Example: Significant figures are in bold	Number of Significant Figures
1	All non-zero digits are significant	**1639.566**	7
2	Zeroes after a decimal point and after a non-zero digit are significant	**11.0** 0.00**50**	3 2
3	Zeroes between non-zero digits are significant	**106**	3
4	Zeroes at the end of numbers punctuated by a decimal point are ambiguous The ambiguity can be removed by reporting the number in scientific notation	**90** 9×10^1 9.00×10^1	1 or 2 1 3
5	When adding and subtracting, your answer needs to have the same number of decimal places as the number with the fewest decimal places	**13.0 + 5.23 =18.2** **14.56** – 0.03 = **14.53** **75 – 5.5 = 70**	1 decimal place 2 decimal places 0 decimal places, but the zero is significant
6	When multiplying and dividing, your answer needs to have the same number of significant figures as the number with the fewest significant figures	**11 × 2** = 20 **5.00 × 7.0 = 35** **2.00/6.0 = 0.33**	1 2 2
7	Exact numbers can be treated as if they have an infinite number of significant figures.	**3.2 × 4 = 12.8**	2
8	Logarithms can only retain in their mantissa the same number of significant figures as there are in the number whose logarithm you are taking.	log (23.75) = 1.376	4
9	When doing more than one calculation, do not round numbers until the end.	**13.2 × 2/5 = 5** (not 6)	1

Table 313 Rules for significant figures

Exercises

1. An object has a mass of 29.1143 g and volume of 25.0 cm^3. Calculate its density.
2. A graduated (measuring) cylinder was weighed three times and the recorded weighings were 12.523 g, 12.497 g, 12.515 g. Calculate the average mass.
3. Determine the volume of a rectangular solid 10.2 cm × 8.24 cm × 1.8 cm.
4. Determine the area of a rectangle 2.1 cm by 3.24 cm.
5. Round off the following numbers to three significant figures: 3.478 m, 4.8055 cm, 5.333 g and 7.999 J.

3.2.2 Plotting graphs and linearising graphs

Plotting graphs

Throughout your IB Chemistry course you will be required to draw and interpret graphs. A graph is a visual representation of data which helps to describe the relationship between two variables.

Your data measurements will frequently involve two types of variables, **dependent** and **independent**. The independent variable is the variable where you, as the experimenter, decide the values. Dependent variables are the results from the experiments.

For example, in an experiment where you observe how the pressure of a gas (at constant temperature) responds to a change in volume, pressure is the dependent variable and volume the independent variable.

When plotting a graph the independent variable is always plotted on the horizontal axis, abscissa or x axis. The dependent variable is plotted on the vertical axis, ordinate or y axis.

When drawing a graph follow these steps:

- Assign the two variables to their correct axes. Time is generally plotted along the horizontal axis since it is usually, but not always, the independent variable. In some experiments IB Chemistry students are asked to find the time taken for a change to occur at various temperatures. The lines of the axes should be ruled with a black line.
- Draw the graph to ensure that the data fill as much of the space on the graph as possible (unless extrapolation is involved. Therefore, choose scales for the x and y axes that cover the range of the experimental data. If both scales start from zero, then the origin should be shown on both axes.
- Your scales do *not* necessarily need to begin with zero at the origin, for example, when constructing an Arrhenius Plot.
- When choosing the scale, always choose values for the major divisions that make the smaller sub-divisions easy to interpret. If an axis must be broken to make best use of the scale, the break should be shown as —//—
- If the graph is used for **extrapolation** then ensure that the range of scales covers the range of the extrapolation.
- Draw a small dot for each data point at the appropriate place on the graph and draw a circle round it for easy detection. If you plot two or more different sets of data on the same set of axes, then encircle the points with different colours for each line. If in monochrome use different shapes, e.g., small circles and triangles.
- The graph should have an informative **title:** simply 'Effect of (independent variable) on (dependent variable)'. Each of the **axes** should be labelled with the name of the variable and appropriate units with a solidus located in between them, for example, Pressure/N m^{-2}. This is to convert the units into pure numbers.

Once the points are plotted they may be joined by a straight line or by a smooth curve (see *Figure 314*), if the chemical theory predicts a smooth, gradual change or transition.

If, however, a smooth, gradual change or linear relationship is *not* predicted from chemical theory, then the data should be joined by short, straight lines. Examples of such graphs include graphs of atomic number against ionisation energy, melting and boiling points. The latter relationship is not common in Chemistry and a frequent student error is to join data points with a series of lines, when a smooth curve is more appropriate.

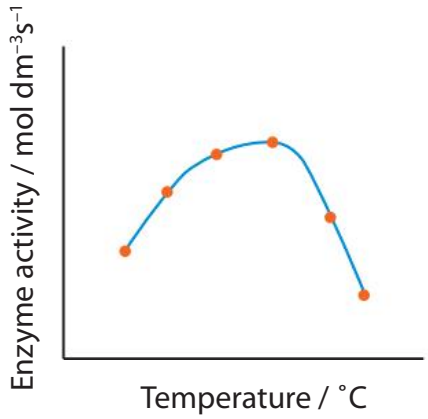


Figure 314 The effect of temperature on the activity of an enzyme

Linearising graphs

Although curved graphs provide information, straight line graphs are more useful and provide more information. So, whenever possible, you should plot data or transformed data that will be expected to produce a straight line or linear graph.

For example, Boyle's law states that the pressure of a fixed mass of an ideal gas is inversely proportional to its volume (provided the temperature is constant). If values of pressure are plotted against corresponding values of volume, a curve will result (see *Figure 315*). It is, however, difficult to assert that the data verify Boyle's law or to 'get a feel' for the accuracy of the data, since widely differing data sets will all give curves when plotted.

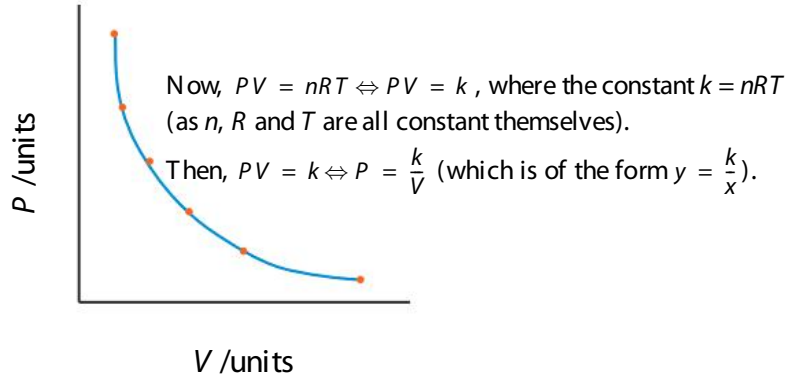


Figure 315 Pressure against volume for a fixed mass of ideal gas (at constant temperature)

An alternative way of expressing Boyle's law is that at constant temperature the pressure of a fixed mass of ideal gas is directly proportional to the reciprocal of its volume. If, therefore, values of pressure are plotted against reciprocal values of volume (V^{-1}), a straight line graph is obtained (see *Figure 316*).

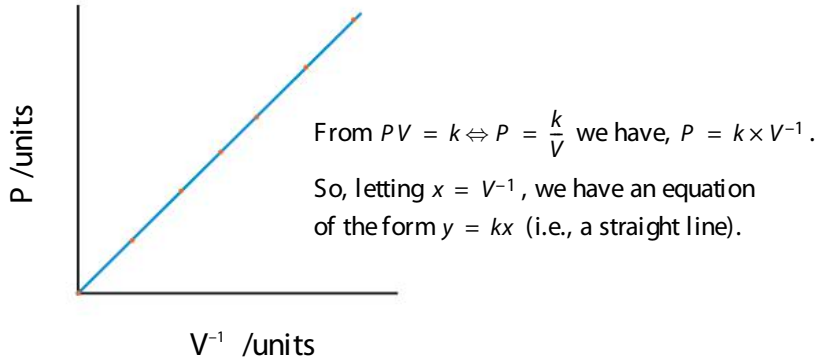


Figure 316 Pressure against reciprocal volume for a fixed mass of ideal gas (at constant temperature)

If the data points plotted from the experimental results do lie on a straight line that runs through the origin, Boyle's law can be said to have been verified. Even when the graph is intended to be a straight line, owing to uncertainties in the experimental results, the points will not all lie on one straight line.

The best straight line is then drawn by drawing a line passing through as many of the points as possible with the points that are not actually on the straight line distributed evenly on either side. A transparent plastic ruler is needed for this task. The resulting line is termed the *line of best fit*. A more accurate approach is to use the *method of least squares* which can be performed using a graphical calculator or the spread sheet Excel.

Sometimes the exact relationship between two variables is not known and it is difficult to decide which transformation should be performed in order to plot data that will produce a straight line graph.

The plot of the logarithm of values of one variable against the logarithm of values of the other variable is often a useful way of overcoming this problem, which may occur during your Individual Investigation.

Thus, if the relationship between the values of the two variables is of the form $a \propto b^n$, we then have that $a = kb^n$

where k is a constant. Taking logarithms (to any base) and rearranging, we have:

$$\log a = \log (k \times b^n) \Leftrightarrow \log a = \log k + \log b^n$$

i.e., $\log a = \log k + n\log b$

Setting y as log a, c as log k

and x as log b

we have $y = c + n\,x$, which is an equation of the form $y = mx + c$, the equation of a straight line (i.e., a linear relationship).

The graph of the values log a on the y–axis against the corresponding values of log b on the x–axis will be a straight line with a slope or gradient of 'm' (i.e., n), (see *Figure 317*).

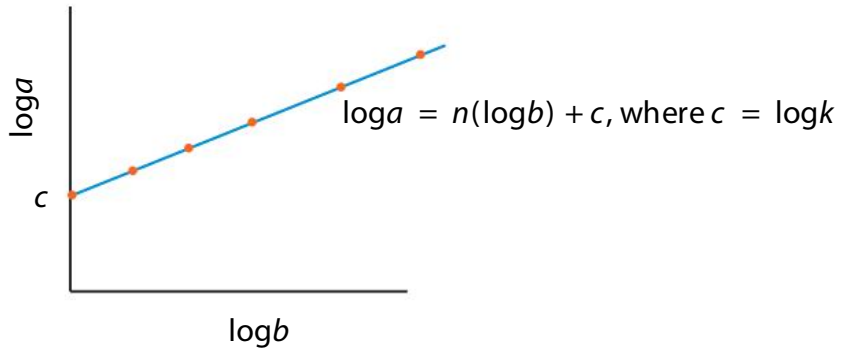


Figure 317 Finding the slope or gradient of a straight line graph

3.2.3 Interpreting graphs

Interpolation and Extrapolation

Sometimes it is necessary to find a value for a variable at a point along the graph that is not one of the original data points.

For example, on the graph below in *Figure 318* we might want to know the volume of gas when the temperature is 75 °C. To determine the volume of gas at 75 °C you must interpolate, or read from the graph between the data points. This is illustrated graphically (see *Figure 318*) where it can be seen that the volume of the gas is 2.3 dm^3 at 75 °C.

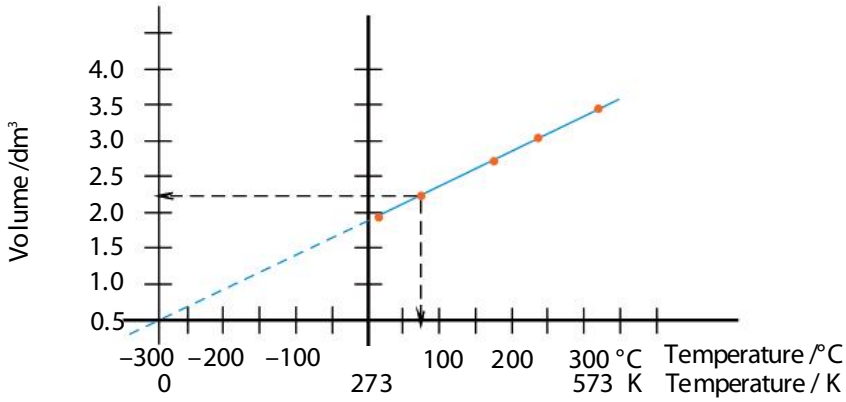


Figure 318 The effect of temperature on the volume of a fixed mass of an ideal gas

If a value is needed beyond the limits of the graph, you must carry out a process called extrapolation. To determine the volume of an ideal gas at –273 °C we must extrapolate, as illustrated by the dotted line, to find the predicted answer of 0 dm^3.

However, you need to be cautious when extrapolating data since the relationship between the variables may not remain the same beyond the limits of your investigation.

For example, real gases will liquefy and freeze to solids before absolute zero (0 K) is reached and will increasingly deviate from the linear or directly proportional behaviour, illustrated in *Figure 318*, as absolute zero is approached. Significant deviations from the Beer- Lambert law arise at high concentration.

Plotting Data

For many graphs the actual raw data or simple averages or means will be plotted. However, if you are plotting data with a known uncertainty or error, of say the average or mean values, then the errors present in the data could be indicated by means of an error bar (*Figure 319*) which represents the known uncertainty or standard error of the mean: 67% of the values used to calculate the mean lie within the error bar. The spreadsheet Excel can be used to plot graphs with the associated error bars to show the random errors (uncertainties).

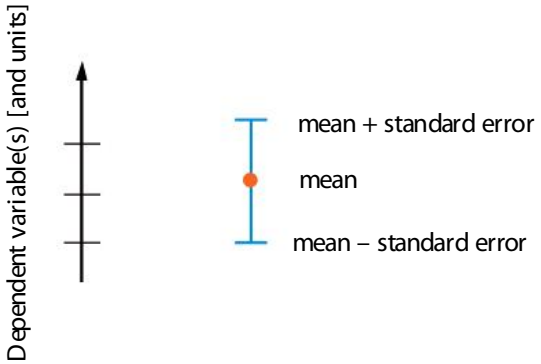


Figure 319 Graph with error bars

When a smooth curve or line is drawn onto the graph it is fitted so that it intersects all or most of the error bars, but not necessarily all of the means. Any curve should be smooth (*Figure 320*) and not a collection of straight lines that 'connect the dots'.

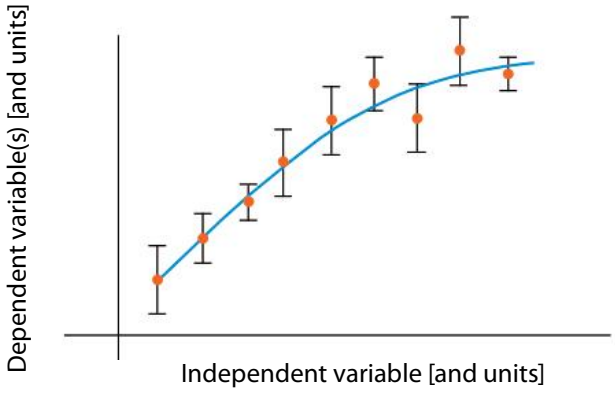


Figure 320 A smooth curve

3.3 Propagation Of Uncertainties

Guiding question:

- *Is the analysis of data accompanied by evidence of an appropriate consideration of uncertainties?*

3.3.1 Calculating uncertainties

The analogue scales on measuring instruments can only be read to some fraction of the smallest scale division. Often this is taken to be half (½) of the smallest division but it may be possible in some cases to estimate a smaller fraction reliably.

The reading uncertainty for instruments with a digital display would normally be taken as ±1 of the smallest change in reading.

When calculations are performed on this data, the random error must be combined or propagated. Using the following rules

RULE 1

If you add or subtract *x* and *y*, the absolute uncertainty in *x*+*y* or *x*-*y* is obtained by adding the absolute uncertainties x and y.

Example

22.34 $cm^3 \pm 0.02\ cm^3$

-1.06 $cm^3 \pm 0.02\ cm^3$

= 21.28 $cm^3 \pm 0.04\ cm^3$

RULE 2

If you multiply or divide *x* and *y*, the fractional uncertainty of *x* times *y* or *x*/*y* is obtained by adding the percent or fractional uncertainties $\Delta x/x$ and $\Delta y/y$.

Percent error can also be calculated for other operations such as squaring etc.

For example,

1.22 g ± 0.01 g

Divided by 21.28 $cm^3 \pm 0.04\ cm^3$

= 0.0573333

= 0.05733 ±0.00058 g cm^{-3}

[(0.01/1.22) + (0.04/21.28)] × 0.0573333 = 0.00058

(leave 2 significant digits in error only)

If the reading is fluctuating, estimate the range over which it is fluctuating. The actual value should be taken as the mid-point of that range, with the associated error being half the range.

Example

If the reading on a balance was fluctuating between 1.017 g and 1.021 g. The value recorded should be ½(1.021+1.017) ± ½(1.021-1.017) = 1.019 ± 0.002 g.

If the reading is stable: The resolution of the display is the smallest amount the display can change by and the error is half of its resolution.

Example

If a display reading was stable (at 1.08) and the smallest the display could change by was 0.01, then the error in the reading would be ± (0.01/2) = ± 0.005.

When spectra are obtained it is typically desired to record the position of peaks on the spectrum, along with their associated error. In such cases, the error should be assumed to equal half the spectrum resolution. The spectrum resolution is the difference between consecutive x-values (at the point where the peak is measured).

A wide variety of questions are listed on the next page to test your familiarity with many of the concepts introduced and discussed in this Chapter.

	Rule	Example
1	When adding or subtracting uncertain values, add the absolute uncertainties	Initial temperature = 34.50°C (± 0.05) Final Temperature = 46.21°C (± 0.05); ΔT = 46.21–34.50 =11.71°C (± 0.05 + ± 0.05 = ± 0.10°C); ΔT should be reported as 11.7 °C ± 0.10
2	When multiplying or dividing add the percentage uncertainties	Mass = 9.24 g ±0.01 Volume = 14.10 cm^3 ±0.05
	(a) Perform calculation	Density = 9.24/14.1 = 0.655 g cm^{-3}
	(b) Convert absolute uncertainties to percentage uncertainties	Mass % error = 0.001/9.24 × 100 = 0.011% Volume % error = 0.05/14.1 × 100 = 0.35 %
	(c) Add percentage uncertainties	0.011% + 0.35% = 0.36 % Density = 0.655 g cm^{-3} (± 0.36%)
	(d) Convert total uncertainty back to absolute uncertainty	0.655 × 0.36/100 = 0.00236 Density = 0.655 g cm^{-3} ± 0.002
3	Multiplying or dividing by a pure (whole) number: multiply or divide the uncertainty by that number.	3.95 kJ ± 0.05 × 10 = 39.5 kJ ±0.5
4	**Powers**: When raising to the n^{th} power, multiply the % uncertainty by n. When extracting the n^{th} root, divide the % uncertainty by n.	$(4.3 \pm 0.5\ cm)^3 = 4.3^3 \pm (0.5/4.3) \times 3$ = 79.5 cm^3 (± 0.349%) = 79.5 ± 0.3 cm^3
5	**Formulas**: Follow the order of operations: find uncertainties for numbers added and subtracted. Use that new uncertainty when calculating uncertainty for multiplication and division portion of formula, etc.	
6	**Graphing** Graphing is an excellent way to average a range of values. When a range of values is plotted each point may have error bars drawn on it. The size of the bar is calculated from the uncertainty due to random errors. Any line that is drawn should be within the error bars of each point. If it is not possible to draw a line of best fit within the error bars then the systematic errors are greater than the random uncertainties (errors).	

Table 321 Rules for error propagation

Exercises

1.

A = 1.0 m ± 0.2 m, B = 2.0 m ± 0.2 m, C = 2.5 m s^{-1} ± 0.5 m s^{-1}, D = 0.10 s ± 0.01 s.

(a) A + B

(b) B–A

(c) C × D

(d) B/D

(e) 3 × A

(f) √(A × B)

2.

The following lengths and associated absolute uncertainties are incorrect. Rewrite them so they are correct.

(a) 9.82 cm ± 0.02385 cm

(b) 10.0 cm ± 2 cm

(c) 4 cm ± 0.5 cm

3.

The accepted value for an enthalpy change is 125 Joules. The experimentally determined value is 150 Joules. Calculate the absolute and percentage errors.

4.

A length is reported as 1.23 m ± 0.04 m. What is the range in which the true value falls? Express the absolute uncertainty as a percentage uncertainty.

Exercises

5.

In an investigation to measure the enthalpy change of combustion of methanol, a spirit burner was weighed, lit and placed beneath a copper can calorimeter holding 200 cm^3 of pure water. The water's volume was measured using a 100 cm^3 measuring cylinder (± 1 cm^3). The density of water is 1.00 g cm^{-3}. After the temperature of the water increased 20.0 °C, the flame on the spirit burner was extinguished. The spirit burner was then re-weighed on an electronic balance (± 0.01 g). The thermometer used to perform the temperature measurements had an error or uncertainty of ± 0.5 °C.

Data Collection

Initial mass of spirit burner	143.45 g
Final mass of spirit burner	142.66 g
Initial temperature of water	19.0 °C
Final temperature of water	37.5 °C

The heat transferred to the water is given by the following expression.

$q = m \times c \times \Delta T$, where m represents the mass of the water in grams, ΔT the temperature rose, represents the specific heat capacity of water (4.18 J g^{-1} $°C^{-1}$) and q represents the heat gained in Joules.

(i) Calculate the amount of heat energy transferred to the water.

(ii) Calculate the mass of methanol combusted.

(iii) Calculate the amount of methanol combusted.

(iv) Calculate the heat transferred by the combustion of one mole of methanol.

(v) Estimate the percentage error in each measurement performed during the investigation. Which is the least precise measurement and hence the greatest source of random error?

(vi) Estimate the percentage error in the enthalpy change of combustion of methanol.

(vii) Suggest other sources of systematic error not considered in the error propagation.

6.

To prepare a solution of sodium hydroxide of concentration 0.050 mol dm^{-3}, 2.00 grams of sodium hydroxide needs to be dissolved to make 1.000 dm^3 of NaOH (aq) solution in a volumetric flask.

The balance used to weigh the sodium hydroxide has a precision of ± 0.005 g and the volumetric flask has a precision of ± 1.0 cm^3.

(i) Estimate the percentage errors in the weighing and in preparing the solution.

(ii) Estimate the percentage error in the sodium hydroxide solution and deduce the absolute error in the solution.

(iii) Identify sources of error in the solution preparation. Assume that the sodium hydroxide used to prepare the solution is not 'fresh'.

3.3.2 Demonstrating uncertainties in graphs

A graph is valuable as it provides a visual impression of the chemical data.

- the existence or not of a trend is easily seen
- data points which do not conform to the general trend are readily identified
- the equation to which a set of data conforms may be suggested by the distribution of the plotted points
- a spreadsheet program, such as Excel, allows graphs to be drawn and data easily analysed
- by including error-bars, an impression can be got of the relative sizes of random uncertainties, from the spread of the points, and of the other sources of uncertainty

It is always worth while drawing a graph of the results whilst the experiment or investigation is in progress. Any data point not conforming to the expected trend can be identified and re-assessed, either by immediately re-doing the measurement, or if this is not possible due to the experimental conditions, then by re-doing that measurement before the equipment is dismantled. Of course, you may not know the expected trend of the graph.

Error propagation in graphs

- Graphs should have a suitable title and a caption in which you describe the contents of the graph. The axes of the graphs have to be labelled with what is measured and unit used.). The independent variable is plotted on the *x* axis and the dependent on the *y* axis.
- Include error bars on each data point. They usually represent the random error or uncertainty in the measurement.
- Draw a line of best fit (this can be done manually by ensuring that there are an equal number of points either side of the line or by Excel as described earlier. This line will represent your experimental results.
- Draw a line of minimal fit (the lowest gradient (slope) that could be drawn that fits your data). Draw a line of maximal fit (the highest gradient (slope) acceptable for your data). (*Figure 322*).
- From the slopes and intercepts of the maximal and minimal lines of fit, determine the range of variation of your line of best fit. Divide the range by 2, and this is the error on your line of best fit. Keep your error to 2 significant figures.

(For example the uncertainty in the slope is one-half of the difference between maximum and minimum slopes).

Figure 322 shows error propagation in a graph where a linear relationship is expected between the voltage of an electrochemical cell and its current.

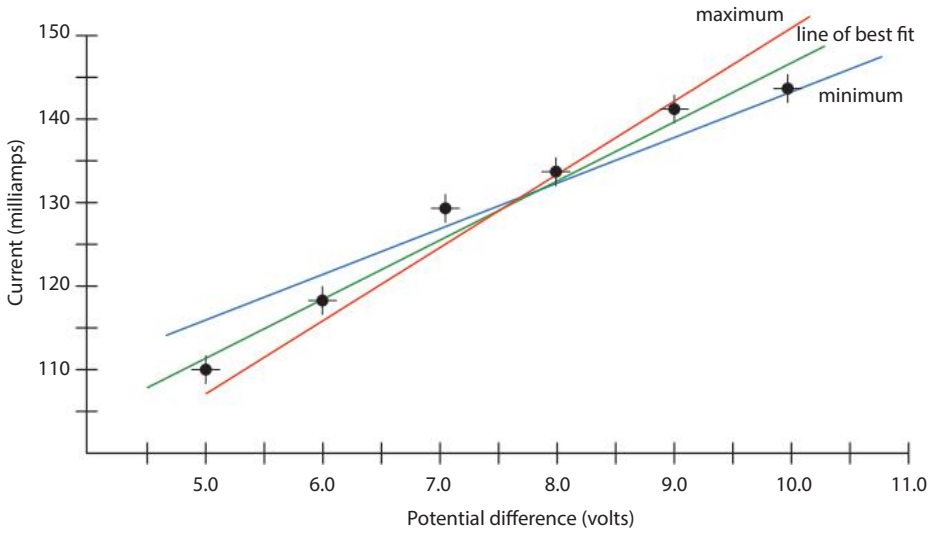


Figure 322 Shows error propagation in a graph

Listed in Figure 323 is a summary of what you need to do to score well in the Analysis criterion.

ASSESSMENT CRITERIA	EVIDENCE REQUIRED	WHAT YOU MUST DO
Recording raw data	Records sufficient and relevant quantitative and associated qualitative raw data	Records sufficient and relevant raw data (qualitative observations and/or quantitative data (usually tabulated). This may include data-logger print outs and digital photographs. Records data for the controlled variables. The data must allow a detailed and valid conclusion to the research question. This often implies data supporting a relationship between an independent and dependent variable.
	Records units and absolute uncertainties where relevant.	Records all measurements to the correct number of significant figures and records appropriate units, usually SI units (showing derivation where appropriate). Records the level of absolute uncertainty or precision for each quantitative reading.
Processing raw data	Processes the quantitative raw data correctly.	Raw data is subjected to relevant calculations (processing). Calculations are correct and accurate to the level necessary. Units are included in the calculations. Significant figures rules are stated and followed. Converts absolute uncertainties to percentage uncertainties and propagates percentage uncertainty calculations correctly. Converts tabulated data into graphical form as relevant. Extracts relevant quantities from the graph (ideally a linear graph) via extrapolation or interpolation or determination of the gradient. Makes an appropriate choice of graph or chart. Simple statistics may be performed if relevant.
	Presents and interprets processed data appropriately and, where relevant, includes errors or uncertainties in calculations and graphs.	• Use of proper scientific conventions in tables (for example, units written once at top of columns), drawings of graphs and charts. • Sample calculations are shown and explained/justified; derived units are included in final calculations. • For graphs, labels and units are correct and scale is appropriate; error bars may be present. • For a graph a line or curve of best fit is drawn (if appropriate). • Final numerical answers are accompanied by an absolute uncertainty.

Figure 323 Details of what is required in the Analysis criterion

This criterion assesses the extent to which the student's report provides evidence of evaluation of the investigation and the results with regard to the research question and the accepted scientific context.

MARK	DESCRIPTOR
0	The student's report does not reach a standard described by the descriptors below.
1-2	A conclusion is **outlined** which is not relevant to the research question or is not supported by the data presented. The conclusion makes superficial comparison to the accepted scientific context. Strengths and weaknesses of the investigation, such as limitations of the data and sources of error, are **outlined** but are restricted to an **account** of **the practical** or **procedural issues** faced. The student has **outlined** very few realistic and relevant suggestions for the improvement and extension of the investigation.
3-4	A conclusion is **described** which is relevant to the research question and supported by the data presented. A conclusion is described which makes some relevant comparison to the accepted scientific context. Strengths and weaknesses of the investigation, such as limitations of the data and sources of error, are **described** and provide evidence of some awareness of the **methodological issues*** involved in establishing the conclusion. The student has **described** some realistic and relevant suggestions for the improvement and extension of the investigation.
5-6	A conclusion is **described and justified** which is relevant to the research question and supported by the data presented. A conclusion is correctly **described and justified** through relevant comparison to the accepted scientific context. Strengths and weaknesses of the investigation, such as limitations of the data and sources of error, are **discussed** and provide evidence of a clear understanding of the **methodological issues** involved in establishing the conclusion. The student has **discussed** realistic and relevant suggestions for the improvement and extension of the investigation.

Guiding Question

- *To what extent has the student demonstrated an understanding of the implications of the conclusion?*

4.1 Formulating the conclusion

Drawing conclusions is a skill that involves analysing the results of a practical and stating and explaining what they show.

Some conclusions are drawn from qualitative observations. For example, the relative oxidising powers of the halogen molecules are seen through their replacement reactions with their halides. The results are then drawn together to show a trend in oxidising power from chlorine to iodine.

Before drawing a conclusion, it may be necessary to do a calculation. It is essential to show the key steps in the working so that the moderator can follow the process and check the accuracy. If there is an anomalous result, then this should not be included in the calculated average. The rules for significant figures should be followed.

Processed results are often shown in graphical form. For example, gradients can be calculated to give initial rates at time zero. These are then plotted on axes of rate (*y*-axis) versus concentration (*x*-axis). When calculating gradients, large triangles should be used to give a more accurate calculation. Graphs are an excellent visual and powerful way of showing trends and relationships.

A straight-line graph shows that there is a directly proportional relationship between the dependent and independent variables. A conclusion should always be supported by evidence from the data and in the case of a directly proportional relationship, the graph should be referred to as providing the evidence. Sometimes graphs are used to find unknown values by using intercepts, coordinates or extrapolation.

When measuring an already known and accepted value of a physical quantity, you should draw a conclusion as to your confidence in their result by comparing the experimental value with the textbook or literature value. The literature consulted should be fully referenced. For example, the literature value for the rate constant at this temperature is 5.6×10^{-3} s^{-1} (*Page 56 in Mechanisms in Organic Chemistry: Case Studies by ROC Norman, MJ Tomlinson and DJ Waddington, Mills and Boon, 1978) (fictitious example only).*

Your conclusions must be supported by the data and are acceptable even if they appear to contradict accepted theories. However, your conclusion must take into account any systematic or random errors and uncertainties. A percentage error should be compared with the total estimated random error as derived from the propagation of uncertainties. In justifying your conclusion, you should discuss whether systematic error or further random errors were encountered. The direction of any systematic errors should be appreciated.

Below is a detailed example of how the identity of an organic acid was logically concluded from a combination of experimental and literature data.

Consider an acid-base titration (*see Figure 401*) whose aim is to determine the molar mass of an unknown diprotic acid, H_2X. The solution of H_2X prepared by the school's technician had a concentration of 28 g dm^{-3}. The student determined the molar mass to be (118 ± 2) g mol^{-1}. The student then performed an Internet search and obtained the following data:

NAME OF DIPROTIC ACID	MOLAR MASS (g mol^{-1})	SOLUBILITY IN WATER (g dm^{-3} at 25 °C)
Butanedioic acid	118.09	5–10
Methylmalonic acid	118.09	Not available
cis-2-butenedioic acid (maleic acid)	116.07	Greater than 100
trans-2-butenedioic acid (fumaric acid)	116.07	Less than 1

Figure 401 Information about organic diprotic acids

(The Internet site URL should be quoted together with the date it was accessed and the authors of the Internet site material).

The solution of H_2X has a concentration greater than both butanedioic acid and *trans*-butenedioic acid. Hence it can be concluded that neither of the two acids is H_2X.

The properties of *cis*-2-butenedioic acid can presumably be explained on account of the intramolecular hydrogen bonding between adjacent -OH groups that takes place at the expense of intermolecular interactions with other acid molecules.

It is assumed that the solution of the H_2X was prepared with a diprotic acid of known solubility, hence suggesting that methylmalonic acid was probably not used.

The concentration of H_2X is within the solubility range of *cis*-butenedioic acid and hence it is likely that *cis*-butenedioic acid is H_2X.

H_2X cannot be an inorganic diprotic acid since the common diprotic acids: sulfuric and carbonic acids have molar masses outside the experimentally determined range.

4.1.1 Establishing the reliability and validity of data

Validity and reliability

Validity refers to the essential truthfulness of a piece of your experimental data. By asserting validity, you are asserting that the data actually measures or reflects the specific phenomenon you claim. Scientific history is full of examples of research findings that were discredited because they were shown to lack validity.

A mercury thermometer is an example of a valid scientific instrument yielding valid data. The height reached by the fluid in an accurate liquid-in-glass thermometer is a valid and appropriate measurement of temperature. Similarly, the movement of a membrane in a barometer is an appropriate and valid way to determine barometric pressure. A ruler can be a valid way to measure length, and an electronic balance can be a valid measure of mass.

Reliability is a different but no less important concept than validity. Reliability relates to your claims regarding the accuracy of your experimental data.

Example

You may claim that the reaction between dilute acid and an iron nail is an exothermic reaction. To test that claim you may out 2 cm of dilute sulfuric acid in a test tube, measure the temperature of the acid (18°C) and add a nail. After about 10 seconds, bubbles of hydrogen form on the nail. After 30 seconds, the mercury thermometer has not registered any temperature change. It is still 18°C. Is your claim wrong?

The assumption behind the procedure is that the iron atoms in the nail will react with the sulfuric acid and release enough heat (thermal energy) for the thermometer to detect it. However, the mercury thermometer chosen may not be sensitive enough to show the temperature change. The more sensitive the measuring device is to changes in the environment, the more accurately you can measure the changes.

You repeat the experiment using a temperature probe and data logger. The probe can detect temperature changes as small as 0.2°C. After about ten seconds the temperature change peaks at 0.4°C. Your laboratory partner repeats the experiment three times, obtains the same result as you and announces that the reaction is, as you predicted, exothermic.

You now have confidence in your conclusion because, by repetition, you have established a consistent pattern of results for the same experiment. Several other students then do the experiment using different probes and data loggers (with the same sensitivity as the one used above) and confirm the pattern of a 0.4°C temperature rise within about ten seconds of the nail being added. More students get involved and a range of thermometers is used to repeat the test.

Three mercury thermometers calibrated to 0.2°C and two alcohol filled clinical thermometers calibrated to 0.1°C can then be used to confirm the results in separate experiments. The consistency of the result from this procedure, regardless of how you measure it, leads you to conclude that the reaction between iron and dilute sulfuric acid is exothermic. The result is a reliable consequence of what you have done, regardless of how you choose to measure it (as long as the measuring device (thermometer) is sensitive enough to allow an accurate measurement of the temperature change to be made). The term reliability refers to the consistency with which you can confirm the result (in this case the temperature change during a chemical reaction).

However, is the above procedure a valid test for the claim that the reaction between the iron atoms of a nail and the hydrogen ions (protons) of a dilute acid is exothermic? That depends on the certainty you have that the source of heat (thermal energy) causing the temperature change is the result of the reaction between the iron atoms from the nail surface and the acid and not from some other chemical reaction. The procedure is valid only if the source of heat in the solution causing the temperature to rise by the amount recorded is the result of a reaction between the iron atoms of the nail and the sulfuric acid.

To be sure, you would have to rule out the possibility that the acid was reacting with a protective coating on the nail. One procedure to sort that out might be to polish the nail with steel wool or fine sandpaper before putting it in the sulfuric acid. To rule out the possibility that the nail (or its coating) is a catalyst for a reaction between the acid and some unknown contaminant in the acid, is more complicated. It would require you to both polish the nail and to find a new source of acid.

When chemical data is collected, quantified or evaluated, reliability refers to the consistency of the measurements; validity refers to whether the measurements you are taking are caused by the chemical phenomena you are interested in. The relationship between reliability and validity can be confusing because measurements can be reliable without being valid. However, they cannot be valid unless they are reliable.

Statistics

Your Individual Investigation may involve large amounts of repeated measurements. If this is the case, then some simple statistical analysis may be appropriate.

A statistical analysis can be performed on experimental data to obtain an uncertainty and confidence in the results, if the distribution that describes the spread in the data points is known. Statistics can be used to quantify the reliability of repeated data.

The most common distribution that describes experimental results is a Gaussian or normal distribution (*Figure 402*), used to represent random processes, such as repeated measurements.

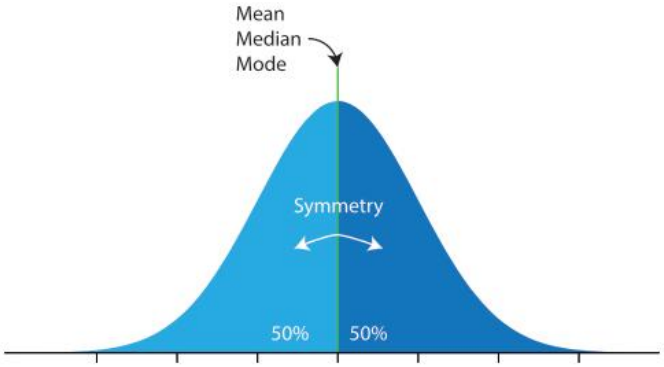


Figure 402 A normal or Gaussian distribution

If an experiment is repeated the (random) variation in the measurements can be used to estimate uncertainties due to random errors.

The mean (average) and standard deviation can easily be calculated (using a calculator), where the mean or average is the best estimate of the true value and the standard deviation is used to calculate the uncertainty associated with the mean (error of the mean, or standard error) by:

error of the mean = standard deviation/sqrt(N)

For similar experiments, the uncertainty associated with each measurement is similar and equal to approximately 1 standard deviation. Repeating the experiment reduces the uncertainty of the mean, however, standard error is a weak function of N so the benefit rapidly decreases as N gets large (maximum of 10 is best).

Exercise

The mass of water delivered by a 5.00-mL pipette was measured in four separate trials. The masses obtained were 4.9871 g, 4.9638 g, 5.0008 g, and 4.9711 g.

Use a calculator to calculate the mean, standard deviation, error and percentage error (take the actual mass of the water as 5.0000 g).

4.2 Evaluation

4.2.1 Evaluating data

Guiding Questions

- *How well has the student justified their choice of research question and approach to the investigation?*
- *To what extent has the student discussed limitations and/or likely sources of error in their methodology?*
- *To what extent has the student discussed the reliability of their data?*
- *To what extent has the student demonstrated an understanding of the impact of experimental uncertainty on their conclusion?*

Evaluation is a skill that students do find difficult to develop. You need to think critically about the reliability of your data and the validity of your conclusions. When developing your skills in this area, a good place to begin is to consider errors.

There are two types of error that affect results as discussed in Chapter 2 (Analysis). Random errors cause results to fluctuate around a mean value and data is made more reliable by averaging repeated readings.

Systematic errors affect all measurements in the same way, producing lower or higher values than the true result. These cannot be averaged out. Sometimes they are due to the particular experimental procedure that has been adopted.

For example, when one student performs a rate experiment it may take time to mix the reagents (sodium thiosulfate and dilute acid) and start the stop clock. This error can be minimised, or even eliminated, by using two students, one to do the timing and one to mix the reagents.

Another source of systematic error may be the measuring device itself. This can be checked by seeing if two different instruments give the same values. For energetics experiments there will be unavoidable heat losses when you are trying to measure an enthalpy change and this causes a systematic error.

You should be looking at experiments and assessing the relative importance of errors in measurement, or in making observations, so that they can judge which sources of error are most important. You should be able to express these errors in a standard format. For example, the measurement of volume of a liquid or solution from a burette may be 21.00 $cm^3 \pm 0.05$ cm^3, while that from an electronic balance may be ± 0.001 g.

In evaluating experiments, you should be able to do the following:

- Suggest improvements to the procedures you adopt.
- Compare repeated results to consider their similarity and thus how reliable they are.
- Identify results that are clearly anomalous.
- Identify variables that you need to control. In some experiments, you need to keep variables constant.
- Estimate uncertainty (random error) in measurements.
- Distinguish between random and systematic errors.

4.2.2 Evaluating methodology

The design and method of your investigation must be commented upon and must not only list the weaknesses but must also appreciate how significant the weaknesses are. Comments about the precision and accuracy of the measurements are relevant here. When evaluating the procedure used, you should specifically look at the processes, use of equipment and management of time.

For example, consider a titration of an unknown sparingly soluble group(II) hydroxide to find its solubility. A titration is performed with aqueous hydrochloric acid of known concentration (given to one significant figure) and phenolphthalein is used as an indicator. The solution of the group(II) hydroxide is filtered prior to the titration.

An evaluation of the procedure should consider the control of temperature since the solubility of solids is often greatly influenced by a change in temperature. The filtrate should be observed for signs of any undissolved group(II) hydroxide–this will be visible as a white suspension. There is always a small systematic error when an acid-base indicator is used and a random error associated with judging the colour change. The precision of the solubility determination is limited by the uncertainty of the standard solution of hydrochloric acid. An unknown error is the manufacturer's purity of the group(II) hydroxide.

Consider a simple investigation into the rate of reaction between marble chips and hydrochloric acid, where the carbon dioxide released is collected above the water in a measuring cylinder (*Figure 403*). The acid was measured using a measuring cylinder.

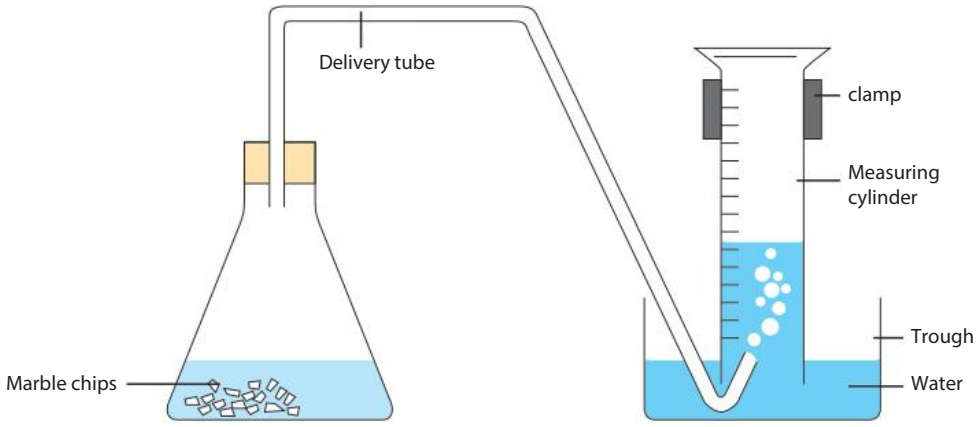


Figure 403 Collecting gas by displacement

Obvious limitations to be mentioned during the evaluation of the methodology are the difficulty in maintaining a constant surface area of marble chips and the use of a measuring cylinder, due its limited precision (which should be quantified). Possible temperature variations should also be suggested as a possible problem during the practical.

4.3 Suggested Improvements

To what extent has the student suggested relevant and feasible modifications to their methodology?

4.3.1 Improving accuracy and precision

Your suggestions for improvement should be based on the weaknesses and limitations identified in Aspect 2. Modifications to your experimental techniques and the data range can be addressed here. Your modifications should address issues of precision, accuracy and reproducibility of the results. You should suggest how to reduce random error, remove systematic error and/or obtain greater control of variables. The modifications proposed should be realistic and clearly specified. It is not sufficient to state generally that more precise equipment should be used.

For example, consider the titration described above. Improvements would include controlling the temperature during the titration by means of a thermostatted water bath in an air conditioned laboratory. Repeating the filtration process and using a finer filter paper to retain more of the excess hydroxide. Hydrochloric acid solution could be made up to a known concentration of more than one significant figure or standardised against a primary standard. The titrations could be repeated and the results averaged to reduce the effect of random errors. The titre due to the presence of the indicator could be established and the titre volumes adjusted to take this into account. Other improvements include using a colorimeter to correctly identify the colour change and using a pH meter to establish the end point.

Summary of the limitations of measurements and experimental procedures

As mentioned previously, many sources of errors arise from the limitations of measurements and experimental procedures. Below is a summary of the various limitations that may be present in an experimental investigation. These should be addressed under the heading Conclusion and Evaluation in the report or 'write-up' for your IB Chemistry Individual Investigation.

Limitations of measurements

- The lack of precision of the instruments used.
- Miscalibration of instruments or apparatus.
- Inconsistency in the recording of measurements.
- Fluctuations in the readings.

Limitations of experimental procedures

- Insufficient or small number of repeats or replicates of measurements.
- The experimental sample (if appropriate to the investigation) was too small.
- The range of the independent variable for a specific investigation was too narrow or too wide.
- The intervals between the values of the independent variable were too large.
- There was a failure to control all the controllable variables.

Assumptions Commonly Made During Investigations Involving Energetics and Electrochemistry

In some experiments it is necessary to make certain assumptions in order to simplify calculations. You will be expected to state these in the written accounts for your IB assessed investigations.

The data tabulated in your IB Chemistry Data Booklet are for standard thermodynamic conditions, that is, 25 °C (298 K) and 1 atmosphere pressure (1.013×10^5 Pa (N m^{-2})). These rarely exist in real experiments, but we frequently assume that we can use the unmodified data from the IB Chemistry Data Booklet.

These standard conditions apply to bond dissociation enthalpies ('bond energies'), enthalpies of formation and combustion, Gibbs energies of formation, lattice energies and acid dissociation constants.

It is also important to recall that bond dissociation enthalpies ('bond energies') quoted in the IB Chemistry Data Booklet are often average values obtained from a range of compounds and only apply to gaseous compounds.

For standard electrode potentials and all thermochemical data involving solutions, there is an additional standard requirement that all solutions (both reactants and products) have a concentration of 1 mol dm^{-3}. Strictly speaking, an activity of one, which takes into account interactions between ions of opposite charge in solution. It is assumed that the activity is equal to the concentration in dilute aqueous solutions, i.e., it is one mol dm^{-3} under standard thermodynamic conditions.

All of the values tabulated in the IB Chemistry Data Book will change if the conditions are non-standard. This can be quantified, but is beyond the scope of the current IB Chemistry program.

A number of assumptions are made for practicals or investigations that involve measuring enthalpy changes using the cooling and heating of water of known mass. In particular the following assumptions are made:

- 1 cm^3 of water has a mass of exactly 1 g; (in fact 1 cm^3 of water has a mass of 0.997 18 g at 20 °C); for dilute aqueous solutions the assumption is even less valid.
- Dilute aqueous solutions behave like water when heated or cooled. In other words, the solutions have the same specific heat capacity as water, namely, 4.18 kJ kg^{-1} K^{-1};
- None of the solution evaporates;

(These three assumptions rarely give rise to significant errors).

- No heat is lost to the immediate surroundings by conduction, convection and/or thermal radiation.

This last assumption gives rise to relatively large errors. These can be reduced by performing the neutralisation or displacement reaction producing the enthalpy change in an insulated container of low specific heat capacity with a lid, or preferably, inside a vacuum flask, though in this case the significant heat capacity of the flask must be determined. Additional heat loss is reduced by using a thermocouple to measure temperature.

- It is important that the heat energy is released quickly, so that the temperature rise in the water reflects the amount of heat produced. If, for example, the reaction under investigation took several hours to go to completion, the amount of heat energy released each minute would be so small that the solution would lose it to the atmosphere almost as fast as it was produced. Therefore, unless the calorimeter was perfectly insulated, the temperature rise and hence the enthalpy change would be underestimated, hence the use of fine powders rather than lumps of solids during thermochemical investigations.
- For the greatest accuracy the temperature change should be as large as measurably possible and centred on room temperature. For example, consider a mercury thermometer that can be read with a precision of ±0.1 °C. Two experiments investigating the same exothermic chemical reaction are performed. The first experiment involves a temperature rise from 20.0 °C to 25.0 °C, while the second experiment involves a temperature rise from 20.0 to 30.0 °C. The first experiment involves an error of ±0.2 °C in 5 °C, a percentage error of 4%, while the second experiment involves an error of ±0.2 °C in 10 °C, a percentage error of only 2%. In practice the temperature rise will often be limited by the concentration of the reagents used.
- Enthalpies of combustion give notoriously poor results if a copper can calorimeter is used. More than half of the heat released warms up the can and the surrounding air, with the latter absorbing the majority of the heat. The accuracy of the procedure can be improved by using a flame calorimeter or a constant-volume bomb calorimeter, (though the latter is outside the current IB Chemistry Programme.)
- Incomplete combustion of an organic substance in air gives rise to carbon monoxide and soot (unburnt carbon), thereby reducing the amount of heat released making the experimental enthalpy change less exothermic than it should be. During such experiments the liquid should be gently stirred to ensure the heat is evenly distributed. However, vigorous stirring should be avoided because it leads to friction and reduces the value of endothermic changes (making them slightly less positive) and increases the value of exothermic changes (making them slightly more negative). However, unless the stirring is very vigorous and prolonged the effect is negligible.

For reactions which are relatively slow, for example, metal replacement reactions involving a metal and metal ions, **extrapolation** needs to be performed as shown in *Figure 404* overpage.

This technique allows you to establish more accurately the maximum temperature rise during the reaction and compensates for heat gains or losses from the surroundings.

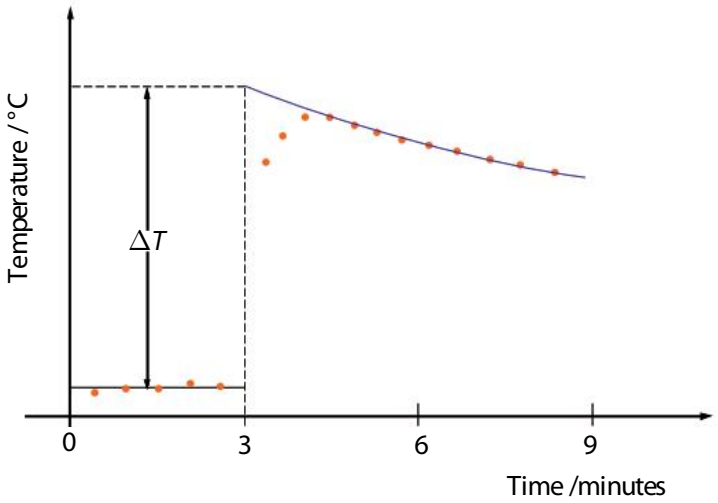


Figure 404 Graph plotted to obtain a corrected temperature change for an enthalpy change whose reaction is initialised at a time of three minutes

Extrapolating the curve back as far as the time at which the reagent was added assumes that the heat loss in the initial stage of the reaction, when the temperature is lower, is the same as the maximum value of the temperature and it would perhaps be better to extrapolate to a time half way between the time of addition and the time at which the maximum temperature is reached.

Investigations Involving Gases

In investigations involving gases, ideal behaviour is assumed; that is, the gas is regarded as a collection of tiny elastic spheres in constant motion. This means that the following assumptions are made:

- there are no attractive intermolecular forces operating between the molecules or inter-atomic forces operating between noble gas atoms and hence there is no tendency for the gas to liquefy at very low temperatures.
- the actual volume of the molecules is negligible compared to the volume occupied by the gas.

In quantitative terms an ideal gas is one that exactly obeys the ideal gas equation or ideal gas law ($PV = nRT$) under all conditions. As a consequence an ideal gas exactly obeys all of the gas laws, namely: Boyle's law, Charles' law, Avogadro's law, the Pressure law and the Combined Gas law. (The preferred description is perhaps Avogadro's hypothesis or principle since it is not a direct summary of experience. It is based on the model of a gas as a collection of molecules behaving ideally).

Strictly speaking, an ideal gas is a hypothetical substance or state that does not exist. However, many gases approximate to ideal behaviour under conditions of high temperature and low pressure. This is particularly true for gases with very weak inter-particle forces, for example, the noble gases. However, gases with strong intermolecular forces, for example ammonia, show greater deviations from ideal behaviour due to the presence of hydrogen bonding, especially at low temperature and high pressure.

However, no gas is an ideal gas and the gases you perform experiments on in the laboratory are described as real gases and do not obey the ideal gas law exactly. Their behaviour is accurately fitted or described by modified gas-law equations that take into account intermolecular forces and the actual volume of the molecules, for example, the van der Waals equation, (which are outside the scope of the current IB Chemistry Programme). It is difficult to quantify the errors in experiments involving gases due to non-ideal behaviour, however, the direction in which they affect the result can often be predicted. They will generally be smaller than experimental errors, for example, loss of gas from the apparatus and lack of precision in the temperature measurement(s).

Investigations Involving Acids and Bases

A number of assumptions are made when dealing with aqueous solutions of acids and bases, namely:

- **Strong acids are completely dissociated or ionised in solution**. In fact, as with all reactions, an equilibrium is established and there will be a small percentage of unionised or undissociated molecules in the solution. The exact amount will vary with the temperature and concentration of the acid. There will also be slight variations in the degree of ionisation or dissociation between hydrobromic, hydroiodic and hydrochloric acids due, in part, to differences in bond strengths. For a strong diprotic acid, such as sulfuric acid, we ignore the second ionisation or dissociation and treat it as a strong diprotic acid. However, for accurate work you should take into account its weak second ionisation or dissociation, but this is not in the current IB Chemistry Programme.
- **For weak acids we assume that dissociation or ionisation is slight** and that only a small percentage of the acid molecules react with water to release ions. This assumption simplifies calculating the pH of the solution from the K_a (or pK_a) and concentration of the acid. A quadratic equation results in a slight increase in accuracy, though this rarely justifies the additional mathematical effort required to solve it. *Use of the quadratic expression is not required by the IB Chemistry Program.*

Two assumptions are made to simplify calculations involving buffer solutions:

- In the buffer solution, the weak acid or weak base dissociation is negligible. This is because the presence of ions from the dissociation of its salt, which will be much greater than that from dissociation, will oppose, and largely prevent, dissociation of the acid or base molecules. (The common ion effect).
- In the buffer solution it is assumed that all of the conjugate acid and base present in the solution are produced by the dissociation of the salt: a negligible amount originates from the acid or base.

Common Assumptions Made About Chemicals and reactions

Assumptions are often made about chemicals, for example, that they are extremely pure, kinetically stable, not readily oxidised or hydrolysed, react according to equations in text books and do not participate in side reactions to form by-products.

Commercial primary standard chemicals (Analytical Reagent (A.R.) grade) are 99.9% pure. The purity of the chemicals you are using will be printed on the reagent bottles. In IB Chemistry work the specification for a primary standard is not usually critical since its purity need only match the accuracy of the apparatus used, please see later in this chapter for how errors due to impurities can be dealt with.

The reactive alkali metals from Group one, such as sodium, have to be stored under oil. Their surfaces are covered with a hard oxide layer that eventually forms sodium carbonate. Magnesium is not stored under oil, but its surface is covered with an oxide layer. Oxide layers can be removed from Group one metals with a scalpel and from other metals with fine sand paper. Lithium differs from the other members of Group one by being covered with a very hard layer of lithium nitride, Li_3N.

Aluminium is a relatively reactive metal, just below magnesium in the reactivity series. However, its true reactivity is 'masked' by a very thin unreactive oxide layer that prevents the underlying aluminium metal from undergoing further oxidation.

Some hydrated salts are not stable in air. Highly hydrated salts, such as sodium carbonate, $Na_2CO_3.10H_2O$, sodium hydrogenphosphate, $Na_2HPO_4.12H_2O$, and sodium sulfate, $Na_2SO_4.10H_2O$, undergo efflorescence, where they lose part or all of their water of crystallisation to the surrounding atmosphere.

$Na_2CO_3.10H_2O\ (s) \rightarrow Na_2CO_3.H_2O\ (s) + 9H_2O\ (g)$

$Na_2SO_4.10H_2O\ (s) \rightarrow Na_2SO_4\ (s) + 10H_2O\ (g)$

The opposite behaviour occurs when substances very soluble in water absorb water vapour from the air to form solid hydrates (hygroscopy) or solutions (deliquescence). Examples of deliquescent substances include anhydrous calcium and iron(III) chlorides, phosphorus(V) oxide, sodium and potassium hydroxide and concentrated sulfuric acid.

Many hydrated salts lose their water of crystallisation upon heating, but at high temperatures thermal decomposition may also occur, for example:

$CuSO_4.5H_2O$ (s) → $CuSO_4$ (s) + $5H_2O$ (g); $CuSO_4$ (s) → CuO (s) + SO_3 (g)

$2FeSO_4.7H_2O$ (s) → Fe_2O_3 (s) + SO_2 (g) + SO_3 (g) + $14H_2O$ (g)

Decrepitation is the violent, noisy breaking up of a salt or other compound when it is heated. Decrepitation often indicates that water is part of the chemical composition of the substance. Such sounds should be recorded as qualitative observations .

The decomposition of hydrated magnesium chloride is complicated by hydrolysis whereby magnesium oxychloride is formed.

$2MgCl_2.6H_2O$ (s) → $MgO.MgCl_2$ (s) + 2HCl (g) + $5H_2O$ (g)

Many organic chlorides and covalent inorganic chlorides, such as anhydrous aluminium chloride, $AlCl_3$, (often incorrectly formulated as Al_2Cl_6 in the solid state) and silicon(IV) chloride, undergo hydrolysis when exposed to moist air.

$AlCl_3$ (s) + $3H_2O$ (l) → $Al(OH)_3$ (aq) + 3HCl (aq)

$SiCl_4$ (l) + $4H_2O$ (l) → $Si(OH)_4$ (aq) + 4HCl (aq)

Such chemicals may therefore have undergone partial hydrolysis if stored for extended periods in opened bottles.

Many metal salts are made by precipitation. For example, zinc chromate(VI) may be prepared by reacting aqueous solutions of zinc sulfate and sodium chromate(VI):

$ZnSO_4$ (aq) + Na_2CrO_4 (aq) → $ZnCrO_4$ (s) + Na_2SO_4 (aq)

However because of the action of co-precipitation and adsorption, small quantities of the other ions present, sodium, chloride or sulfate, will be present in any salts prepared or manufactured in this way. This tendency is greatly increased when the precipitate formed is basic in character.

In addition, during storage, salts 'age': they lose small amounts of water and form small insoluble residues. Many metallic oxides when stored for long periods under ordinary laboratory conditions become contaminated with their carbonates.

Many apparently simple chemical reactions often involve side reactions. For example, the combustion of magnesium in air to form magnesium oxide is accompanied by two side reactions, namely:

3Mg (s) + N_2 (g) → Mg_3N_2 (s)

2Mg (s) + CO_2 (g) → 2MgO (s) + C (s)

The combustion of sodium and potassium in air or oxygen provide another examples of side reactions accompanying an inorganic reaction. In addition to the oxides, sodium peroxide and potassium superoxide are formed.

2Na (s) + O_2 (g) → Na_2O_2 (s)

K (s) + O_2 (g) → KO_2 (s)

Side reactions will also be observed during metal displacement reactions. For example, during the reaction between zinc and aqueous copper(II) sulfate, small amounts of hydrogen gas will be evolved due to the acidic nature of hydrated copper(II) ions.

$[Cu(H_2O)_6]^{2+}$ (aq) → $[Cu(H_2O)_5OH]^+$ (aq) + H^+ (aq)

Zn (s) + $2H^+$ (aq) → Zn^{2+} (aq) + H_2 (g)

Side reactions may also occur during the electrolysis of aqueous solutions using graphite (carbon) electrodes. Significant amounts of carbon monoxide and carbon dioxide may be formed, due to oxidation of the anode at which oxygen is being liberated.

Some chemicals are photosensitive and undergo partial decomposition in the presence of sunlight (which contains ultraviolet radiation). Examples include the silver halides, chloric(I) acid (present in 'chlorine water') and concentrated nitric(V) acid:

$2AgX\ (s) \rightarrow 2Ag\ (s) + X_2$ (where X is a halogen)

$2HClO\ (aq) \rightarrow 2HCl\ (aq) + O_2\ (g)$

$4HNO_3\ (l) \rightarrow 2H_2O\ (l) + 4NO_2\ (g) + O_2\ (g)$ (simplified)

Organic reactions are notorious for the presence of significant side reactions. A classic example concerns nucleophilic substitution reactions which are always accompanied by the major side reaction of 1,2-elimination.

This is exemplified below with bromobutane:

Substitution: $C_4H_9Br\ (l) + OH^-\ (aq) \rightarrow C_4H_9OH\ (l) + Br^-\ (aq)$

Elimination: $C_4H_9Br\ (l) + OH^-\ (alc) \rightarrow C_4H_8\ (g) + H_2O\ (l) + Br^-\ (alc)$

These reactions occur simultaneously since the hydroxide ion can act as both a nucleophile (an electron pair donor that reacts with an electron deficient carbon atom (this is a better definition of nucleophilicity than vague notions about seeking out nuclei or centres of positive charge) and a base (a proton acceptor).

However, the following factors are known to favour elimination:

- the presence of an ethanolic ("alcoholic") solvent.
- the reactant being a tertiary halogenoalkane (R_3CX).
- the presence of an alkene type double bond or benzene ring in the 'halogeno' compound.
- a high temperature (the entropy change, ΔS, becomes more favourable).

Moreover, many organic reactions are accompanied by rearrangement reactions and the production of carbon particles via a charring process, especially if concentrated sulfuric acid is employed. A final complication for many organic reactions is that they do not go to completion and the products will therefore be contaminated with reactants.

These examples stress the importance of carrying out some research into reactions that you are using or investigating during a piece of internally assessed IB Chemistry coursework. It may be necessary to consult specialised inorganic or organic Chemistry Textbooks.

Assumptions Made for Performing Titrations

The following conditions should be met when performing a titration:

- One of the reactants in the titration should be a standard or should be capable of being *standardised*, that is, having its concentration in mol dm^{-3} established by titration with a standard solution .
- The reaction should proceed to a stable and well defined *equivalence point*, where there are stoichiometric quantities of the reactants.
- The end point and hence the equivalence point must be detectable. This is usually either by means of a colour change involving the reactants or products or via the presence of an indicator. Alternatively, a pH probe and meter or conductivity probe and meter can be used to detect pH or conductivity changes.
- The reaction must proceed by a known and definite pathway. There should be no competing side reactions.
- The reaction should be virtually complete at the equivalence point, i.e., the chemical equilibrium should overwhelmingly favour the products. The chemical equilibrium constant, K_c, should be relatively large.
- The reaction rate should be fast enough to be practical, otherwise a *back titration* should be carried out. Slow approaches to equilibrium can cause erroneous judgments about reaction completeness.

Assumptions made during gravimetric analysis

Gravimetric analysis involves establishing a chemical formula or purity of a compound via a series of weighing processes. Reactions suitable for gravimetric analysis include: reactions between elements to form compounds (so-called direct syntheses), the decomposition of hydrated salts and precipitation reactions.

(Examples of such reactions and their associated calculations can be found in Chapter 1 of *Chemistry (for use with the International Baccalaureate)* 4th Edition by *John Green* and *Sadru Damji*).

Gravimetric analysis generally takes longer than titrimetric analysis, but is more accurate because of the use of a sensitive electronic balance which has a higher degree of precision than volumetric glassware.

There are several points to be considered when designing or carrying out a gravimetric analysis:

- There must be a phase change so that the product can be separated from the reaction solution. In practice this means that either the product is a solid precipitated from solution, or is an evolved gas, leaving a solid product.
- The reaction must be essentially complete. For precipitation from solution, this is achieved when the solubility product, K_{sp}, is small. In cases of sparingly soluble solids an excess common ion should be present in the solution to reduce solubility of the salt. It also means that there are no competing equilibria that might re-dissolve the product.
- The final product must be pure and must be of a definite chemical composition.
- The rate of reaction must be fast enough to fit in with time constraints.

Errors in Gravimetric Analysis

You may be expected to know the effect of various types of random and systematic errors on a gravimetric analysis. For problems like this, one approach (apart from intuition) is to make up some fictitious (contrived) numbers and see how the various changes affect the final result.

A worked example is now given: an IB Chemistry student analysed a sample of hydrated copper(II) sulfate to determine the amount of water of crystallisation by weighing the sample and heating it to convert it to anhydrous copper(II) sulfate. The theoretical or accepted value of the percentage of water by mass is 32%.

Deduce the effect of the following errors on the experimentally determined value for the percentage of water by mass.

1. After the sample was weighed, a small piece of rust fell from the tongs into the crucible

Let us imagine the initial mass of the hydrated copper(II) sulfate was 30 g and that after heating to constant mass the final mass was 20 g: a loss of water of 10 g.

The percentage of water would therefore be $\frac{10}{30} \times 100$, that is, approximately 33%.

If a piece of rust (which will not evaporate or decompose) is added, then the final mass would be higher than expected, for example, 25 g (the rust had a mass of 5 g). Inserting this new value into your equation, you will find that your percentage of water is now $\frac{30 - 25}{30} \times 100$, that is, approximately 17%, a value lower than expected. An error of this type thus has the effect of producing an experimental result that is below the accepted value of 32%.

2. Moisture driven from the sample as steam condensed on the inside of the crucible cover

The initial mass of the hydrated copper(II) sulfate would be unchanged. However, instead of leaving the crucible, the water would be retained on the cover of the crucible, thereby making the final mass too high. Assuming 5 g of water condensed on the crucible lid, you will find again that your percentage of water is now $\frac{30 - 25}{30} \times 100$, that is, approximately 17%, a value lower than expected. An error of this type thus has the effect of producing an experimental result that is below the accepted value of 32%.

3. The original sample of hydrated copper(II) sulfate contained a proportion of anhydrous copper(II) sulfate

The initial mass would remain unchanged, but the final mass would be higher than expected because you would not be losing all of the water that you would have done if the sample was pure hydrated copper(II) sulfate.

Thus $\frac{30 - 25}{30} \times 100$ still gives 17%, a value lower than expected.

4. The original sample of hydrated copper(II) sulfate was wet

30 g of the sample will be weighed out, but more mass would be lost during the heating process than would be expected, making the final mass, for example, 5 g. This gives $\frac{30 - 5}{30} \times 100$ that is, 83% water by mass. This is a value higher than the accepted value.

Errors due to Impurities

The purity of the reagents may also be taken into account during an analysis. For example, if 1.000 dm^3 of 1.000 mol dm^{-3} NaCl(aq) (M = 58.44 g mol^{-1}) is to be prepared for a titration involving precipitation, and if the sodium chloride is supplied as 99% pure (i.e., 99±1)%, then you should use 59.03 g of sodium chloride rather than 58.44 g (assuming the impurities do not react similarly to sodium chloride) since:

Mass of commercially supplied sodium chloride (NaCl) = $\frac{100 \times 58.44}{99}$ = 59.03 g

The ±1% uncertainty in the composition of the sodium chloride should be combined with the uncertainties from the mass and volume measurements in calculating the acceptable range of the sodium chloride concentration.

Standard solutions

Solutions used in acid-base and redox titrations whose concentrations are known to a high degree of accuracy and whose concentrations do not appreciably change with time, are known as standard solutions.

A chemical suitable for the preparation of standard solutions for use in titrations should have the following properties. It must:

- be available in a highly pure dry state.
- be stable in air and not undergo oxidation or hydrolysis (i.e., can be weighed without any special precautions).
- be readily soluble in water and give a stable solution that does not readily undergo reduction, oxidation or decomposition (either spontaneously or via hydrolysis with water).
- titrate reproducibly in a known reaction and not undergo side reactions.

- have a large molar mass to reduce the effects of any small errors or uncertainties in weighing, thus improving the accuracy of the concentration of the solution (see below for a worked example).

A solution is required that contains 0.02 mol of a chemical in 250 cm^3 of a solution. The balance being used to weigh the chemicals is accurate only to ±0.01 g.

You have two substances, A, with a molar mass of 20.00 g mol^{-1}, and B with a molar mass of 200.00 g mol^{-1}.

Mass of A required = 0.02 mol × 20.00 g mol^{-1} = 0.400 g

Mass of B required = 0.02 mol × 200.00 g mol^{-1} = 4.00 g

Consequently,

Percentage error in weighing out A = $\pm\frac{0.01\ g}{0.400\ g} \times 100 = \pm 2.5\,\%$

Percentage error in weighing out B = $\pm\frac{0.01\ g}{4.00\ g} \times 100 = \pm 0.25\,\%$

Observe that the percentage error involved in the weighing is directly proportional to the molar mass: an increase in the molar mass by a factor of ten, decreases the percentage error or uncertainty by a factor of ten.

One reagent unsuitable for the preparation of standard solutions is potassium manganate(VII) (permanganate) which is difficult to prepare pure, and slowly oxidises water to oxygen converting itself to manganese(IV) oxide (manganese dioxide). This oxidation of water is accelerated by light and heat. It is catalysed by manganese(II) ions and manganese(IV) oxide.

$4MnO_4^-\ (aq) + 4H^+\ (aq) \rightarrow 4MnO_2\ (s) + 2H_2O\ (l) + 3O_2\ (g)$

This reaction is particularly rapid if the solution is acidified (and the pH is less than 3). Potassium manganate(VII) solution is only stable in the presence of free alkali, that is, in solutions in which the pH value is greater than 7.

Iron(II) salts readily undergo aerial oxidation where the surfaces of solutions or crystals slowly react with water and oxygen in the air to form iron(III) salts. This can be inhibited in aqueous solution by acidifying the solution.

Anhydrous sodium and potassium hydroxides (especially the former) are deliquescent and absorb water vapour and carbon dioxide from the air. Their solutions slowly absorb carbon dioxide from the air forming dilute solutions of the corresponding carbonate thereby making them unsuitable for the preparation of standard solutions.

For example: $2NaOH\ (aq) + CO_2\ (g) \rightarrow Na_2CO_3\ (aq) + H_2O\ (l)$

Chemicals suitable as Primary Standards

Chemicals suitable for the preparation of standard solutions include:

A. Primary redox reagents

- (Hydrated sodium thiosulfate)
- Potassium dichromate(VI)
- Potassium iodate(V)
- Potassium bromate(V)
- Iodine (in the form of iodine dissolved in aqueous potassium iodide)
- Hydrated ethanedioic (oxalic) acid

Standard solutions of sodium thiosulfate are not usually made by weighing alone because there is some uncertainty about the degree of hydration in the hydrated salt and the solutions cannot be kept for long periods of time since they are photosensitive and susceptible to bacterial decomposition.

B. Primary acids

- Phthalic acid (1,2-benzenedicarboxylic acid) (in the form of potassium hydrogen phthalate – "KHP")
- Hydrochloric acid (constant boiling point (azeotropic mixture))
- Sulfamic (aminosulfonic) acid
- Benzoic (benzenecarboxylic) acid
- Hydrated disodium tetraborate (borax)

C. Primary bases

- Anhydrous sodium carbonate

It is important to use boiled distilled water to make up standard solutions for use in acid-base titrations. The boiling process removes much of the dissolved carbon dioxide present in distilled water. If not removed it will participate in the titration and reduce the accuracy of the titration calculation.

D. Precipitation titrations

- Silver nitrate
- Sodium chloride

E. Complexometric titrations

- EDTA (Ethylenediamine tetra-acetic acid) (disodium salt, dihydrate)

Chemicals unsuitable as Primary Standards

Substances **not** suitable as primary standards include:

- Sulfuric acid
- Sodium hydroxide

They absorb water from the air. Sodium hydroxide also absorbs carbon dioxide and forms sodium carbonate. A standard solution of sodium hydroxide can be prepared if nitrogen gas is passed through the distilled water to remove dissolved carbon dioxide, prior to the addition of sodium hydroxide. Sodium hydroxide also slowly dissolves the silica present in glass.

- Nitric(V) acid decomposes on storage and because it is a strong oxidising agent causes undesirable side reactions
- Potassium manganate(VII) decomposes on storage
- Iron(II) compounds oxidise in moist air

Indicators

Acid-base indicators (*Figure 405*) are usually weak acids and will participate in acid-base titrations. It is therefore important that the indicator be highly coloured and that excessive amounts are not used during a titration. *(Litmus is not a single substance and should only function as an indicator for a strong acid-strong base titration).*

The pH range of an acid-base indicator is usually about 2 pH units. However, the assumption that a ratio of one to ten in concentrations of the two indicator forms for complete colour masking is not

INDICATOR	COLOUR CHANGE	pH RANGE
Bromothymol blue	Yellow /Blue	6.0–7.6
Litmus	Red/Blue	5.8–8.0
Methyl red	Red/Yellow	4.2–6.3
Methyl orange (screened)	Green/Purple	2.9–4.6
Phenolphthalein	Colourless/Red	8.3–10.0
Phenol red	Yellow/Red	6.8–8.4
Methyl orange	Red/Yellow	3.1–4.4

Figure 405 Common indicators

always true. If you examine *Figure 303* you will see that pH ranges vary somewhat. It is possible to obtain a sharper colour change in a titration using a mixture of an indicator and an inert dye. An example is screened methyl orange in which a blue dye is added to methyl orange to make the colour change more obvious.

If the solution is being used to establish a titration curve the presence of aqueous carbon dioxide ('carbonic acid') will make experimental end points less sharp than expected, and can lead to pH changing with time near the end point as the equilibrium between aqueous carbon dioxide and 'carbonic acid' (hydrogen and hydrogen carbonate ions in equilibrium) establishes itself relatively slowly. Carbonic acid also acts as a buffering agent.

The end point of a titration occurs when the indicator is recognisably all the final colour, that is, the term 'end point' refers to the indicator. The equivalence point, however, refers to the stoichiometry, that is, when there are exactly equivalent amounts of the reactants and neither is present in excess. The indicator must be carefully chosen so that the colour change occurs as close to the equivalence point as possible.

When an indicator is used, the colour change may occur at a pH which is not the equivalence point pH. The end point may differ from the equivalence point, perhaps because an unsuitable indicator has been used, or because the indicator itself significantly affected the volume of titrant needed.

The first type of error can be minimised through careful indicator selection; the second type, by performing a blank titration (all chemicals, except the unknown solution or solid, present). Blank titrations indicate what volume of titrant is needed to just change the colour of the indicator alone. This volume, known as the titration or indicator error, is then subtracted from any volumes obtained from titrations with the unknown solution or solid.

If the analyte (the substance under analysis), titrant (the standard solution) or products of the titration reaction have distinctive colours, the titration may be 'self-indicating'. This is the case, for example, with redox reactions involving potassium manganate(VII).

In redox titrations involving potassium manganate(VII), this reagent is usually placed in the burette. (In the titration of nitrite (nitrate(III)) ions, to prevent loss of nitrogen dioxide during the titration, acidified aqueous potassium manganate(VII) solution is placed in an evaporating basin and the solution of sodium nitrate(V) run in. As soon as nitrous acid (nitric (III) acid) is formed, it is oxidised.

The reagent is intensely purple, and when it reacts in acidic aqueous solution it turns colourless. The end point is when the titrating reagent is in excess, so the reaction mixture will (just) turn pale pink. The reason for placing it in the burette is so that the colour change from colourless to pale pink is easier to see than the reverse, namely, pink to colourless.

If starch is being used as an 'indicator' during a redox titration involving iodine then it should be added near the end point, that is, when the solution takes on a 'straw' or pale yellow colour, and **not** at the beginning of the titration. If added too early, the indicator forms an insoluble blue complex with the iodine. This will not dissociate when thiosulfate ions are added. The titre will therefore be too low.

In titrations, silver nitrate solution is used to determine the concentration of chloride ions. In order to establish the end point potassium chromate(VI) is used as an indicator. Chromate(VI) ions give a red precipitate of silver chromate(VI) with silver ions. However, silver chloride is more insoluble than silver chromate(VI), so if silver ions are added to a solution containing a mixture of chromate(VI) ions and chloride ions, it is silver chloride that is precipitated first. The end point is therefore when the colour of the precipitate turns from white to pink. Potassium chromate(VI) does not work in an acidic solution since it is converted to dichromate(VI) ions, so the indicator is destroyed. If a chloride solution is acidic, calcium carbonate powder can be added to neutralise the acid.

It is very important to record observed colour changes when performing a titration.

Common student mistakes are:

- the initial colours of the reactants and indicators are not recorded.
- the colour change occurring in the indicator is not specified.
- the colour change at the endpoint of a titration is given the wrong way round.
- 'clear' does not mean 'colourless'.

The accurate recording of the colours obtained during an acid-base titration is important. For example, methyl orange changes colour from yellow in alkaline solutions to red in acid solutions via an orange transition-colour, which is generally taken as the end point.

If a solution of acid is standardised by one student against sodium carbonate using the *orange* end point and then a second student uses this acid titrant to titrate a sample using the *red* end point, then the second student's result will be inaccurate since the molar concentration of the acid titrant is based on the orange end point.

Before using a titrant standardised by someone else, find out what end point was used during the standardisation. If you are in doubt then re-standardise the solution yourself.

If hydrochloric acid of (unknown concentration) is going to be standardised against an aqueous solution of sodium carbonate solution (a primary standard), one of two indicators may be employed: screened methyl orange or phenolphthalein.

However, note that they detect different end points:

Na_2CO_3 (aq) + 2HCl (aq) → 2NaCl (aq) + CO_2 (g) + H_2O (l) Screened methyl orange

Na_2CO_3 (aq) + HCl (aq) → $NaHCO_3$ (aq) + NaCl (aq) Phenolphthalein

Back Titrations

Back titrations are used when insoluble solids, for example, bases, need to be analysed. The problem with the conventional titrations is that the solid base reacts rather slowly with dilute acid, and so gives a drawn out end point. In back titration the insoluble base is dissolved in excess acid, after which the excess acid is reacted rapidly with a standardised solution of alkali, giving a sharp end point.

Consider a back titration to determine the purity of magnesium hydroxide using 100 cm^3 of 1.00 mol dm^{-3} hydrochloric acid solution. The amount of hydrochloric acid must be more than enough to react with all the magnesium hydroxide.

$Mg(OH)_2$ (s) + 2HCl (aq) → $MgCl_2$ (aq) + H_2O (l)

The amount of hydrochloric acid is 0.10 mol. $\left(1 \times \frac{100}{1000}\right)$

Hence the amount of magnesium hydroxide to be taken for analysis should be less than 0.05 mol.

If 0.04 moles of magnesium hydroxide are used the mass is 2.32 g. (0.04 × (24 + 32 + 2)).

This method would work well if the magnesium hydroxide were contaminated with magnesium chloride, an inert substance that does not react with hydrochloric acid.

However, the method would not well if the basic contaminants, for example, magnesium oxide and other group II hydroxides or carbonates, were present.

Contaminants with a lower molar mass would cause the purity of the magnesium hydroxide to be greater than 100%, for example, magnesium oxide, MgO.

$Mg(OH)_2$ (s) + 2HCl (aq) → $MgCl_2$ (aq) + H_2O (l)

= 2.32 g $Mg(OH)_2$

= 0.04 mol

MgO (s) + 2HCl (aq) → $MgCl_2$ (aq) + 2H_2O (l)

= 2.32 g MgO

= 0.058 mol

$$\text{Amount} = \frac{\text{mass (g)}}{\text{molar mass (g mol}^{-1})} = \frac{2.32}{(24+16)} = 0.058 \text{ mol}$$

Both compounds react in a 1:2 molar ratio with hydrochloric acid, but magnesium oxide has a lower molar mass than magnesium hydroxide. Hence a given mass of magnesium oxide would react with more acid than the same mass of the hydroxide. Conversely reactive contaminants with a higher molar mass (such as magnesium carbonate) would lead to a result that was less than 100%, but still greater than the true purity. The hydrochloric acid could be replaced by sulfuric acid concentration of 0.5 mol dm^{-3} since magnesium hydroxide reacts in a 1:1 molar ratio with sulfuric acid, so sulfuric acid of half the concentration could be employed.

Replacement reactions

Below is an outline of how to approach the Evaluation criterion. For example, consider again the replacement reaction between zinc powder and an excess of aqueous copper(II) sulfate solution. Assume that the data obtained confirm (within experimental error) that there is a directly proportional relationship between the masses of zinc and copper and a graph with line of best fit has been drawn.

The graph shows that as the mass of zinc is increased, the mass of copper produced also increases. In fact if the mass of zinc is doubled then the mass of copper also doubles. This can be shown from the lines drawn on the graph. When the mass of zinc is increased from 1.0 g to 2.0 g the mass of copper produced doubles from 1.52 g to 3.04 g. This means that they are directly proportional or in a linear relationship. This experiment proves, within experimental error, that if the mass of zinc is doubled, then the mass of copper produced also doubles.

This is because one atom of zinc will replace one atom of copper. If appropriate, relate your answer to your initial hypothesis, for example, this proves my original hypothesis that the mass of zinc is directly proportional to the mass of copper.

Compare your results, if appropriate, to literature values obtained from a text-book, data book from the reagent bottle, Internet or from your IB Chemistry teacher. Calculate out how close as a absolute and percentages your values agree. Comment on to what extent your results agree. If you calculated some theoretical or predicted values in your hypothesis, then you could also compare your answer to these.

Any assumptions should be identified. For example, the calculation assumes that the copper(II) sulfate solution and the zinc powder are 100% pure. The temperature and time are assumed to be sufficient for the reaction to go to completion and that the reaction is irreversible. It is assumed that the law of conservation of mass is exactly obeyed.

Consider human, chemical and equipment errors and limitations. If your answer is greater or lower than the literature or theoretical values then try to specifically explain in your discussion regarding errors why this might be.

For example, if the experimental masses of copper are consistently above the theoretical values then the reasons for this could be that the surface of the copper slowly oxidised in air to form copper(II) oxide whilst drying. This will increase the mass of copper and also explains why it became darker in colour since copper(II) oxide is black. Perhaps the copper was not completely dry and so the mass was increased due to the water present. Some of the copper(II) sulfate may have crystallised on the filter paper and so this contributed to an increase in mass. Perhaps the temperature and time were insufficient for the reaction to go to completion. Copper(II) sulfate solution is slightly acidic, so perhaps the zinc was reacting with hydrogen ions to release hydrogen in a side reaction. Perhaps some copper passed through the filter paper.

Suggest relevant improvements and modifications that can produce more accurate and reliable results. Although you can suggest trying to improve precision with more repeats and to improve reliability with more independent values, try also to be specific and make these relevant to the specific systematic errors and limitations previously discussed.

For example, dry the moist copper for a longer period sealed with a dehumidifying agent (for example, dry silica gel) and in the absence of air, to make the copper drier and also to ensure that it is not oxidised. Use more finely divided zinc to ensure that the reaction is faster because more of the zinc is exposed to the copper(II) ions. Use better pre-heated quality filter paper (folded into a fluted shape) that allows less solid copper to pass through. Carry out a control experiment by passing copper(II) sulfate through the filter paper and drying it. Calculate by how much the mass of the filter paper changes and subtract this value from each of the answers.

4.2.2 Extending the investigation

Guiding question

- *To what extent has the student suggested relevant and feasible extensions to the investigation?*

Extending the investigation may involve the choosing of a new independent variable, a new dependent variable or a new methodology.

Wines have a low pH because they contain a mixture of weak organic acids. The main ones are tartaric, malic, lactic and acetic acids but small quantities of citric and succinic acids may also be present from the grapes used to prepare the wine.

For example consider an individual investigation that involves the titration of white wine to determine the total acidity of opened white wine against time by titrating it against a solution of 0.10 mol dm^{-3} sodium hydroxide. Suitable indicators include phenolphthalein or a 1:1 mixture of phenol red and bromothymol blue.

Extending the investigation may involve changing from white wine to red wine. The red pigments (mainly anthocyanins) will need to be removed by activated charcoal. The charcoal can be removed by simple filtration.

Alternatively, you could use a pH meter and plot a curve of pH against the volume of alkali added for the white wine (or red wine that has been decolourised).

Some of the weak acids contribute to what is known as the volatile acidity of the wine, while the rest are responsible for what is called the fixed acidity. You can separate the volatile and non-volatile acids by steam distillation. Titrating the steam distillate and/or evaporated residue will enable you to find out how much of the wine's acidity is volatile and how much is fixed.

Exercise

The Faraday Constant can be determined from the following experiment. It is the charge in coulombs carried by one mole of electrons. It involves electrolysing copper(II) sulfate solution using copper electrodes.

The reaction at the cathode is reduction: Cu^{2+} (aq) + $2e^-$ →Cu (s).

The reaction at the anode is oxidation: Cu (s) →Cu^{2+} (aq) + $2e^-$.

The cathode (negative electrode) is cleaned and weighed before being placed in the copper(II) sulfate solution. The current is maintained at 0.30 A for 40 minutes. The cathode is removed from the electrolyte and carefully washed with distilled water to remove any copper(II) sulfate solution. Distilled water is removed from the cathode by rinsing it with propanone. The cathode is finally dried by allowing the propanone to evaporate from its surface. The cathode is reweighed and placed back in the solution. A constant current of 0.30 A is passed for a further 40 minutes when the rinsing, drying and weighing are repeated. This procedure is repeated a further 8 times.

Time/minutes	Mass of cathode/g	Mass of copper deposited/g	Time/s	Charge/C
0	115.75			
40	115.98			
80	116.22			
120	116.47			
160	116.71			
200	116.95			
240	117.20			
280	117.50			
320	117.68			
360	117.93			
400	118.15			

(a) Use the additional columns of the table to record the charge passed and the mass of copper deposited on the cathode. [charge in coulombs = time in seconds × current in amps].

(b) Calculate the Faraday constant and present the data in graphical form {mass of copper deposited (*y*-axis) against charge passed (*x*-axis)} and draw a line of best fit.

(c) Indicate clearly one anomalous point on the graph that you did not use when drawing the line of best-fit. By reference to the instructions for the experiment suggest an explanation for the anomaly.

(d) The balance used by the student weighed to 2 decimal places. By reference to the results of the experiment explain why it would have been more appropriate to use an analytical balance weighing to 4 decimal places.

Listed in Figure 406 is a summary of what you need to do to score well in the Evaluation criterion.

Assessment criteria	Evidence required	What you must do
Concluding	States a conclusion, that is described, justified and supported by the data.	Analyse and explain the data from the experiment and draws a valid conclusion which is relevant to the research question and its scientific context (background information that may include a hypothesis, competing hypotheses and a scientific model). The conclusion must be supported by the raw and processed data, (though it may be tentative and subject to some statistical uncertainty). If a graph is present, the correct graphical relationship is stated and numbers quoted to support the relationship. The graph may be used to obtain a gradient or intercept or be used for extrapolation or interpolation. If appropriate, uses the graph to identify any anomalous data points. Where appropriate, compares the experimental result with the accepted result: calculates absolute and percentage errors from the expected or literature value. Compares results obtained by repetition, or against the chemical literature, and comments on the reliability of the values obtained. Some simple statistics may be included if large numbers of repeated random measurements are recorded.
Evaluating methodology and data	Evaluates strengths and weaknesses, such as limitations of data and sources of error	Outline any limitations to the accuracy/reliability/amount/range of data that you have obtained. States simplifying assumptions that were made which may affect the accuracy of the results. Discusses any limitations of the methodology used. Identifies and quantifies limitations due to the precision and accuracy of the equipment. Performs error propagation with random errors. Identifies possible systematic errors or other unanticipated factors. Strengths may involve control of variables, reduction of random errors and identification of systematic errors. Weaknesses may involve inability to control or monitor important controlled variables, biological variation, large random errors or large percentage errors in small measurements.
Improving and extending the investigation	Suggests realistic improvements in respect of identified weaknesses and limitations.	Suggests modifications to improve the existing investigation to reduce random errors and to identify possible sources of systematic error. Suggests alternative methodology to improve the investigation, perhaps by better control of controlled variables and more precise measurements of the dependent variable. Suggests alternative equipment or apparatus (with higher sensitivity) if applicable. Suggests how to extend the experiment, for example, collecting additional and more precise data outside the current data range.

Figure 406 Summary of the Evaluation criterion.

This criterion assesses the extent to which the student's report provides evidence that the student has selected, recorded, processed and **interpreted** the data in ways that are relevant to the research question and can support a conclusion.

This criterion assesses whether the investigation is presented and reported in a way that supports effective communication of the focus, process and outcomes.

MARK	DESCRIPTOR
0	The student's report does not reach a standard described by the descriptors below.
1-2	**The presentation of the investigation is unclear, making it difficult to understand the focus, process and outcomes.** The report is not well structured and is unclear: The necessary information on focus, process and outcomes is missing or is presented in an incoherent or disorganized way. The understanding of the focus, process and outcomes of the investigation is obscured by the presence of inappropriate or irrelevant information. There are many errors in the use of subject specific terminology and conventions e.g. incorrect/ missing labelling of graphs, tables, images; use of units, decimal places. For issues of referencing and citations refer to the academic honesty section.
3-4	**The presentation of the investigation is clear. Any errors do not hamper understanding of the focus, process and outcomes**. The report is well structured and clear: the necessary information on focus, process and outcomes is present and presented in a coherent way. The report is relevant and concise thereby facilitating a ready understanding of the focus, process and outcomes of the investigation. The use of subject specific terminology and conventions is appropriate and correct. Any errors do not hamper understanding.

Guiding questions:

- *To what extent is the student work concise, clear, and structured in a logical sequence?*
- *How well does the reporting of the methodology allow the investigation to be successfully repeated by others?*
- *How well does the report allow the process of data analysis to be followed?*
- *How well does the report allow the process of data analysis to be followed?*
- *To what extent is appropriate subject-specific terminology used throughout the investigation?*
- *To what extent is appropriate subject-specific notation used throughout the investigation?*
- *To what extent has the student used correct conventions for presentation of quantitative data, including appreciation of decimal places, significant figures, and uncertainties where appropriate?*

5.1 Organization of the written report

The following is a suggested layout for the written report for the Individual Investigation. It is *not* mandated by the IBO and other presentations may also be acceptable.

5.1.1 Formatting a report

Title

List the title of the experiment or meaningful name for your research report, for example:

To investigate paramagnetism in transition metal salts.

This could be in the form of a cover page that also includes your full name (as registered with the IBO), your school's name and your IB candidate number.

Contents page

The contents page will list the contents and page numbers for ease of cross-referencing. All pages must be numbered throughout the report. Hotlinks to the pages may also be useful.

Abstract

The best way to learn how to write a good abstract is to read published abstracts from chemical journals, for example, the *Journal of the American Chemical Society* (JACS) (*Figure 501*).

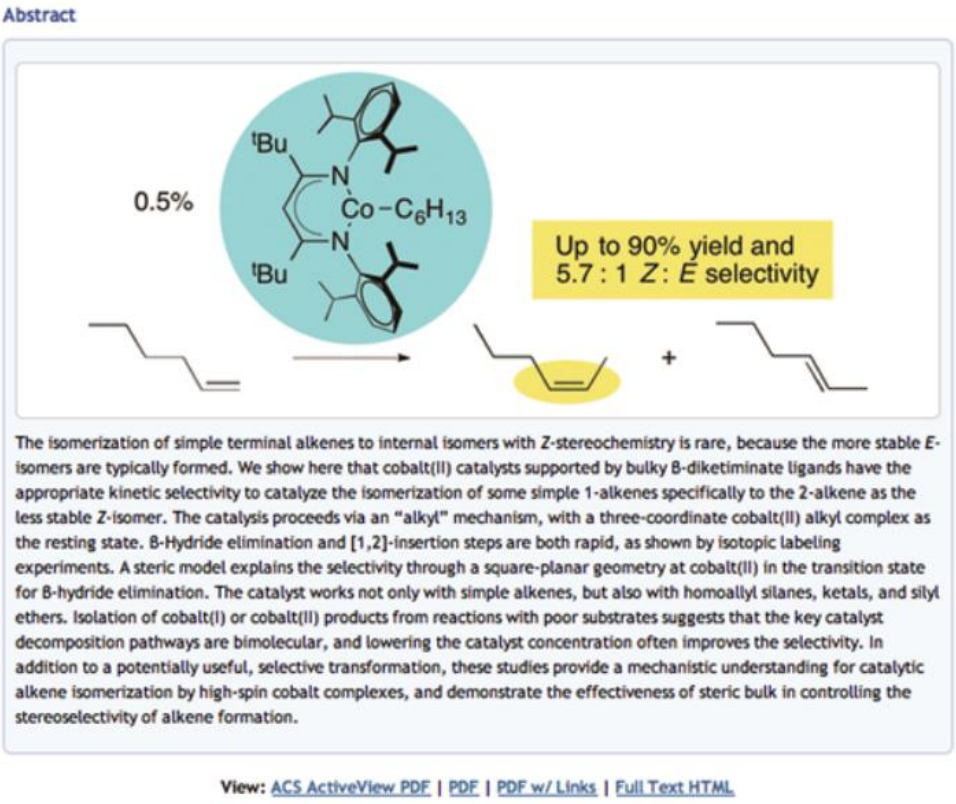


Figure 501 An on-line abstract from JACS <http://pubs.acs.org/doi/ipdf/10.1021/ja408238n>

The abstract should 'stand alone' which means that one of your peers should be able to read only your abstract and understand the basic nature of the report for your Individual Investigation. For this reason, a good abstract clearly identifies the purpose of the investigation and the important results.

Avoid comments such as, '*This experiment helped me learn about the nature of organic chemical reactions*' or '*The goal of this experiment was to learn about complexes between EDTA and transition metal ions.*' Although those are important aspects and goals of the lab experience, the research report should focus only on the data and results. Avoid starting your abstract with, '*The purpose of this investigation was.....*'

Background information on the chemical theory or applications of your investigation belongs in the Introduction section. Avoid referencing any other sources or parts of the report, because the abstract should 'stand alone.'

Be specific about what was done: name the chemical reagents or types of instruments that were used, the products of a reaction, numerical values that were measured or calculated, etc. But do not be too detailed: volumes and concentrations are probably not necessary in the abstract.

Avoid vague statements such as '*A metal complex was prepared and the percent yield was calculated.*' A better abstract would read '*hexaammine nickel(II) fluoride was prepared from nickel(II) fluoride, ammonia, ammonium chloride and hydrogen peroxide. The yield was 8.45 g (64 % based on nickel).*'

Introduction

The introduction section explains what focused chemical research question is being addressed. It includes general background material and a brief historical perspective on the topic being investigated. It presents brief summaries, with references, of previous work. Any relevant chemical laws, theories, models and hypotheses must also be included. An effective introduction directs the person reading from a larger area of chemical research, through examples of progress in that chemical field to a clear statement of the research question and approach being addressed in the Individual Investigation Report. Diagrams, structural formulae, balanced chemical equations, etc. must be included as appropriate.

Downloading directly from the Internet or copying directly from books may suggest to your Teacher and the IB moderator that you have not understood the chemistry involved and may be considered as plagiarism. It is always best to put everything into your own words.

Method

The experimental section should provide all the necessary detail for someone to be able to reproduce your work and obtain the same results (within experimental error). There should also be a 'Planning' section you explain what various options were open and why one technique was chosen rather than an alternative.

Often in a chemical paper a chemical experimental section is subdivided into Materials (sources and purity of reagents used), Preparation of Compounds (with procedure, and summary of characterization by NMR, IR, UV-Vis spectroscopy, melting point, chromatography) and Instrumentation (manufacturer, description of any adaptation or sample preparation) sections.

This approach may or not be appropriate for your Individual Investigation report, but the guiding principle here is reproducibility.

Results

This section should include a summary of your raw data (preferably in tabular form) and important observations (qualitative data). Major calculations may be included in this section, or in as separate Interpretation section or in an Appendix. A description of the mathematical equations used in your calculations must be presented.

All quantities should have units and be expressed using the correct number of significant figures and decimal places and random uncertainty. Scientific notation should be used when appropriate. For values less than unity, use a leading zero. Avoid writing values having too many zero; use scientific notation. Error propagation must be performed.

Examples

'0.15 cm^3' not '.15 cm^3'

'2.5×10^{-5} mol dm^{-3}' not '0.000025 mol dm^{-3}'

Important experimental conditions should be listed as footnotes, especially when the table includes data obtained under different experimental conditions. All tables, figures and graphs should be numbered sequentially and must be mentioned in the text.

Discussion

A discussion section should take the form of an analysis of your results and whether you have answered your research question.

Comment on the purpose of the experiment. What do the results indicate? What are sources of random and systematic error (experimental uncertainty/precision)? What additional experiments could help address any unresolved issues? Do the results agree with what other researchers have found? Do the results support a chemical model or hypothesis?

Conclusion

Summarise your results and discussion with a short conclusion that is more than simply a repetition of your results. Phrase it in terms of the research question addressed in the Introduction.

References

Citations of the literature used in the previous sections.

Appendices

Photographs of the apparatus and results may appear here, along with lengthy mathematical or statistical calculations or additional material not needed when reading through the report, e.g. preparation of solutions or buffers. The risk assessment and safety information, e.g., CLEAPSS hazcards or MSDS data sheets may also appear in the Appendix.

4.1.2 Sentence style and writing style

The following guidelines are designed to improve the quality of your reports for experimental work and bring it close to the standard of a published chemical paper. The key guiding principle is clear communication. You will *not* lose any marks for poor English phrasing unless the meaning is unclear or incorrect. The IBO is aware that many IB Diploma students have English as a Second Language (ESL).

Beginning a sentence

Avoid beginning a sentence with a symbol, numeric value or equation.

Incorrect:

317.8 mg of sodium chloride was added to the solution, which was then heated to 55 °C by means of a thermostatted water bath.

Correct:

After the addition of 317.6 mg of sodium chloride, the solution was heated to 55 °C by means of a thermostatted water bath.

Dangling Modifiers and Illogical Construction

Check that a modifier phrase or the pronoun 'it' actually refers to the intended subject.

Incorrect:

After transferring to a larger round bottomed flask, the solution of benzoic acid was heated to a boil.

Correct:

The solution of benzoic acid was transferred to a larger round bottomed flask and heated to a boil.

Equations

Mathematical equations typically appear in italics as a separate line from the text and are numbered sequentially throughout the manuscript. Equations can then be referred to by number.

$\frac{Q}{zF} = n$, where F is the Faraday constant, z is the ion charge, Q is the electric charge and n is the amount of substance discharged.

Spaces

There should be one space between a quantity and its units and between a quantity or word and subsequent parenthetical phrase.

6.626 kJ

25.15 K = 298.15 °C

45 cm^3

456 nm

(34,000 M^{-1} cm^{-1})

Personal pronouns

By tradition, scientists avoid using the personal pronouns 'I', 'we' and 'you' in most scientific communications. The use of third person instead of first person is preferred when reporting results.

First person: *I heated the solution of the dye at 100 °C for 1 hour and I noticed that it turned pale red.*

Third person: *When heated at 100 °C for 1 hour, the dye solution turned pale red.*

Subject-verb agreement

Based on whether the subject is singular or plural, use the correct verb tense. A quantity used is a singular subject, even when that quantity is in a plural form of units.

Incorrect: *1.20 g of solid sodium hydroxide were added …*

Correct: *1.20 g of solid sodium hydroxide was added …*

Ensure you are not stating that an inanimate object is drawing a conclusion, or suggesting a strange cause and effect.

Incorrect: Water was present in the crude aspirin product because of the peak at 3200 cm^{-1} in the IR spectrum. (*the peak in the IR spectrum did not cause water to be present*)

Correct: The peak at 3200 cm^{-1} in the IR spectrum indicates that water was present in the aspirin product. (the *water caused the peak in the IR spectrum)*

'Verbing' a noun

Do not turn nouns into verbs.

Incorrect: *ammonia complexes to copper(II) ions*

Correct: *ammonia forms complexes with copper(II) ions*

Incorrect: *the reaction mixture was centrifuged to separate the colloidal sulfur*

Correct: *the colloidal sulfur was separated from the reaction mixture using a centrifuge*

Tested

A hypothesis can be 'tested' but for most laboratory work, the terms 'measured,' 'investigated,' 'determined,' 'calculated' or 'obtained' often work better.

Incorrect: The absorbance of the solution was tested using the UV-vis machine

Correct: The absorbance of the solution was measured using a UV-vis spectrophotometer.

Abbreviations, Formulas and Numerals

Use standard abbreviations, for example, h = hour, min = minute, s = second and °C = degrees Celsius.

Chemical formulas and names

Use subscripts, superscripts, parentheses, and symbols appropriately in chemical formulae.

Examples:

Fe^{3+} (aq), NaBr (s) and $K_2[PtCl_4]$.

IUPAC names should be used:

Examples:

$CuSO_4.5H_2O$ (s) copper(II) sulfate-5-water

C_6H_5COOH benzene carboxylic acid

Chemical names should not be capitalized unless trade names, e.g., Paracetamol.

Defining abbreviations

Abbreviations for chemical compounds (e.g. tris), ligands (e.g. EDTA), instruments (e.g. IR) or methods should be defined in the text before using throughout the report for your Individual Investigation. However, this is a minor issue and is the practice of published scientific papers.

5.2 Referencing

Referencing is a standardised method of acknowledging the sources of information you have consulted for writing your Individual Investigation report. Words, paragraphs, quotes, figures, tables, theories, ideas, facts–originating from another source and used in your Individual Investigation report must be referenced (i.e. acknowledged). Referencing is done for the following reasons:

- to avoid plagiarism.
- so that your Assessor can verify quotations.
- so that your Assessor can follow up on the original author's thinking by consulting the source you used.

There are many ways to acknowledge sources of information, for example, MLA (Modern Language Association), and none is mandated by the IBO. This publication recommends a Bibliography at the end of the Individual Report together with in-text referencing. The style adopted is the MLA (Modern Language Association) format. However, what is important is that the method used is consistent. Do not switch from one method to another. Familiarise yourself with the format and terms (*Figure 502*) that your school or IB Chemistry teacher expects you to use.

Paraphrasing	This is explaining in your own words what the original source wrote.
Quoting	"To repeat (words) exactly from (an earlier work, speech or conversation), usually with an acknowledgement from the source" (Collins Paperback English Dictionary, 1998, p. 665) Put in quotations everything that comes directly from the text especially when taking notes. (Collins Paperback English Dictionary, 1998, p. 136).
Citing or In-Text Referencing	"1. To quote or refer (a passage, book or author). 2. To bring forward as evidence" When citing your sources, you are telling your IB Chemistry Teacher who/what the original source. You are giving credit where credit is due.
Bibliography	This is a list of cited works.
Common Knowledge	These are facts that are located in several sources and probably known by many chemists.

Figure 502 Important referencing terms

Terms to Know

In-text referencing

In-text referencing is when you provide information about the source in the text of your Individual Investigation report. The bibliography at the end of your report shows the reader which sources were researched but sometimes that is not enough. That is when you use in-text referencing **inside** your essay. Usually the author's last name and a page reference are enough to identify the source. With this information, the reader can find the complete publication information in your citation list at the end of your essay.

Tips for in-text referencing

When you find a useful resource for your Individual Investigation Report, note down all the details required in your bibliography (e.g. author, title, publication details, date of access, URL etc) before you start taking notes.

When reading a resource highlight key words, main ideas or make bullet point notes that you might want to include in your essay.

If you use the exact words from the writer put them inside quotation marks so you do not accidentally plagiarise, and if possible note down the page number.

Examples of In-Text Referencing

Signal Phrase: introduces where the idea or quote comes from and usually has the author's name in the text.

According to Anthony *Methylacidiphilum fumariolicum* SolV bacterium, a methanotroph (methane consumer) found in Italian volcanic mudpots, relies on lanthanides to survive (Anthony 68-69).

Signal phrase = According to Anthony

Paraphrase or Summary: the idea in your own words or the main ideas only.

Current research has shown that certain species of bacteria that metabolise methane found in Italian volcanic mud need rare earth metals (lanthanides) to survive.

Direct Quote: show these are the exact same words used by the author in the source with quotation marks.

'This fascinating work has important implications for studies of most other methanotrophs growing on methane or methanol' (Anthony 47).

Citation in Bibliography: this is the source with the full publications details.

Homewood, Jon "The effect of global warming on amphibians". New Scientist. 1 October 2009: 38-41.

Because Internet sources typically have no page or paragraph numbers, and Web sites often list no author, students are often confused about how to refer to these sources within their papers. The answer is to cite the author's name whenever possible, and use the source's title otherwise (or a shortened version of the title). If no page or paragraph number is provided, leave that portion of the citation blank. Keep in mind that the primary purpose of an in-text citation is simply to point readers to the correct entry on the "Works Cited" page. Also, as web sites change, give the date it was referenced so, if necessary, cached versions may be retrieved.

Bibliography

How to cite sources

Books

Author's name (put family name first). Title. Place of publication: Publisher, Year of Publication.

Note: titles can be underlined or put into italics

e.g.: Andrew, John. Chemistry in Focus. United Kingdom: Hodder and Stoughton, 1999.

Two authors (note the order of names for the second author)

McKissack, Patricia, and Frederick McKissack. Modern Biology. United Kingdom: Oxford University Press, 1995.

Three or more authors

Adams, Roger *et al.* Encyclopedia of Science. New York: Consolidated Press, 1994.

Encyclopedia article

Article title". Title of Encyclopedia. Year of Publication.

Note: put title of article in speech marks

e.g.: "Ozone layer". World Book Encyclopedia. 2009.

Interview

Name of the person interviewed. The kind of interview (personal, telephone, email). Date or dates of interview.

e.g.: Martin, J. K. Email interview. 8-12 May 2008.

Magazine Article

Author. "Article title". Magazine title. Date of Magazine: Pages.

Note: the use of speech marks and underlining

e.g.: Churchman, Deborah. "Global warming: the sceptic's view". New Scientist.March1999: 28-31.

Remember also that:

- citations should not be numbered.
- citations should not be separated into different formats (e.g. books, websites, interviews, etc.).
- citations should be in alphabetical order by the main entry (e.g. author's surname, title, article title, etc.). Ignore a, an, the.

Website

Author (if available). "Title of the article." (in speech marks) Title of whole site. Date of visit to site. *<URL of Page>*.

e.g.: "Using MLA Format." Purdue University Online Writing Lab. January 23, 2006. *<http://owl.english.purdue.edu/handouts/research/r_mla.html>*

Online Encyclopedia Article

Author. (family name first) "Title of article". Magazine title . Date of Magazine: Page numbers. Product Name. Date researcher visited site. *<Electronic Address, or URL, of the source>*.

e.g.: Churchman, Deborah. *"Be a Nature Detective"*. Ranger Rick March 1999: 28-31. MasterFILE Premier on-line. EBSCO Publishing. 30 Feb. 2004.

<http://www/epnet.com/ehost/login.html>.

There are several on-line bibliography makers. Try them out but you are advised to use the MLA version and take care with the data you enter otherwise you will get a bad outcome. Try Landmarks Citation Machine and Bibme.org for example:

<http://citationmachine.net/>

<http://www.killerstartups.com/Web20/bibme-org-the-quickest-way-to-build-a-bibliography>

Additional Materials for Writing Lab/Research Reports

Davis, Martha *Scientific papers and presentations* San Diego: Academic Press, **1997**

Dodd, Janet S. (ed.) *The ACS style guide: a manual for authors and editors* ACS, **1997**.

Eisenberg, Anne "Strategies five productive chemists use to handle the writing process." *J. Chem. Educ.* **1982,** *59,* 566.

Potera, Carol "The Basic Elements of Writing a Scientific Paper: The Art of Scientific Style" *J. Chem. Educ.* **1984,** *61,* 247.

Spector, Thomas "Writing a Scientific Manuscript: Highlights for Success" *J. Chem. Educ.* **1994,** *71,* 47.

5.3 Use of units

SI Base Units

The six basic quantities or base units of the SI system commonly used in Chemistry are: the metre for measuring length, the kilogram for measuring mass, the second for measuring time, the mole for measuring the amount of substance, the kelvin for measuring temperature and the ampere for measuring electric current (*Figure 503*).

Dimension	Symbol	SI unit name and symbol
Length	*L*	metre, m
Mass	*m*	kilogram, kg
Time	*t*	second, s
Temperature	*T*	kelvin, K
Amount of substance	*n*	mole, mol
Electric current	*I*	ampere, A

Figure 503 The six commonly encountered physical quantities in chemistry

One physical quantity that is very important in Chemistry, is volume, which is derived from length and expressed in metres cubed, m^3. However, the usual unit used in Chemistry is the decimetre cubed (1 dm^3), which is commonly called a 'liter' in North America (symbol L) and 'litre' in Europe. There are 1000 dm^3 in one metre cubed (1 m^3). Each decimetre cubed (dm^3) can be divided into 1000 centimetre cubed (cm^3). Note that milliliter (mL) is widely used in North America and can be virtually regarded as being identical to cm^3 (1 litre = 1.000028 dm^3).

Strictly speaking, measurements of length should be expressed in metres and masses of chemicals should be expressed in kilograms. However, often such measurements are expressed in centimetres (cm) and grams (g), where 100 cm = 1 m and 1000 g = 1 kg.

The size of the units given above is not always the most suitable for certain measurements and decimal multiples and fractions are frequently used as shown below. A set of common SI prefixes and associated symbols is given in *Figure 504*.

Fraction	Prefix	Symbol	Multiple	Prefix	Symbol
10^{-1}	deci	d	10^{3}	kilo	k
10^{-3}	milli	m	10^{6}	mega	M
10^{-6}	micro	μ	10^{9}	giga	G
10^{-9}	nano	n	10^{12}	tera	T

Figure 504 SI Factors

SI Derived Units

A large number of additional SI units exist and are widely used during the IB Chemistry Program, for example, the joule for energy. The joule and other so-called derived units can be expressed in terms of base units.

Commonly used SI derived units and their symbols for a number of physical quantities relevant to the IB Chemistry program are given below in *Figure 505*, together with a 'useful' relationship between these and the definition in terms of SI base units. (The term specific in front of a physical quantity has the meaning 'per unit mass').

Quantity	Definition	Unit	Relationship to other quantities	Basic definition
Molar concentration (formerly molarity, M)	mole per decimetre cubed	mol dm^{-3}		mol dm^{-3}
Frequency	reciprocal second	Hz		s^{-1}
Wave number	reciprocal metre	m^{-1}		m^{-1}
Volume	metre cubed	m^3		m^3
Force	newton	N	J m^{-1}	kg m s^{-2}
Energy/Enthalpy	joule	J	N m	kg m^2 s^{-2}
Entropy	joule per kelvin	J K^{-1}		kg m^{-2} s^{-2} K^{-1}
Gibbs free energy change or enthalpy change	joule per mole	J mol^{-1}		kg m^2 s^{-2} mol^{-1}
Molar entropy	joule per mole per kelvin	J mol^{-1} K^{-1}		kg m^2 s^{-2} mol^{-1} K^{-1}
Pressure	pascal	Pa	N m^2, J m^{-3}	kg m^{-1} s^{-2}
Charge	coulomb	C		A s
Potential difference (voltage)	volt	V	J s^1 A^1	kg m^2 s^{-3} A^{-1}
Density	kilogram per metre cubed	kg m^{-3}		kg m^{-3}
Heat capacity	joule per kelvin	J K^{-1}		kg m^2 s^{-2} K^{-1}
Specific heat capacity	joule per kilogram per kelvin	J kg^{-1} K^{-1}		kg m^2 s^{-2} kg^{-1} K^{-1}

Figure 505 SI derived units and their symbols

The base and derived SI units are a **coherent** system of units. This means that all the units for the derived physical quantities are obtained from the base units by multiplication or division without the need for the introduction of numerical factors. This simplifies many chemical calculations.

For example, if we consider the ideal gas equation, $PV = nRT$, we can rearrange it to make P the subject, namely,

$$P = \frac{nRT}{V}$$

We can then substitute numerical values for the volume of gas (V), the amount of gas (n), the molar gas constant (R) and the absolute temperature (T), in coherent SI units, namely, m^3, mol and J K^{-1} mol^{-1}, respectively and calculate the numerical value of P which will also be in coherent SI units, namely pascals.

Example

If R = 8.31 J K^{-1} mol^{-1}, T = 300 K, $V = 6.34 \times 10^{-3}$ m^3 and n = 0.250 mol.

Then,

$$P = \frac{nRT}{V} = \frac{0.250\ \text{mol} \times 8.31\ \text{J K}^{-1}\ \text{mol}^{-1} \times 300\ \text{K}}{6.34 \times 10^{-3}\ \text{m}^3} = 9.83 \times 10^4\ \text{Pa}$$

Note that the more familiar unit of volume the decimetre cubed is not a base or fundamental SI unit and would not yield a pressure in pascals.

Rules For The Use of SI units

1. Units may be written out in full, e.g. 5 coulomb, or by using the agreed symbol, e.g., 5 C, and printed in upright Roman type.
2. A full stop is not written after symbols, except at the end of a sentence.

3. Values of quantities are expressed in SI units using Arabic numerals (i.e. 1, 2, 3,… etc) and the symbols for the units. e.g., m = 5.0 g but not m = five gram or m = five g.
4. A space should be inserted between the numerical value and the unit's symbol. e.g., a 5.00 g copper cube but not a 5.00g copper cube.
5. The digits of numerical values having more than four digits on either side of the decimal marker can be separated into groups of three using a space. e.g., 15 739.012 53 is better than 15739.01253
6. Avoid abbreviations, such as sec (for either s or second) or cc (for either cm^3 or centimetre cubed).
7. Avoid mixing unit symbols and unit names, for example, kg/m^3 or, better still, kg m^{-3} is acceptable, but not kilogram/m^3.
8. Those symbols named after a person have a capital for the first letter. When the name of the unit is written in full it has a small letter, even when commemorating a person, for example, pascal, symbol Pa.

Common Mistakes with SI Units

- The rules listed previously may seem minor at best, and at worse pedantic, but it is good practice to follow them. Below are outlined some major and common mistakes frequently made by IB Chemistry students.
- It is not acceptable to record measurements with a mixture of units, for example, 5 min 10 s and 1 kg 10 g. These should be expressed as 310 s and 1.01 kg, respectively.
- Another common mistake is to confuse weight and mass. When using a chemical balance masses should be recorded in kilograms (kg) or grams (g). Weight is a force (due to gravity) and should therefore be expressed in newtons (N). On Earth a l.0 kg mass has a weight of approximately 9.8 N. (Weight on Earth varies slightly according to latitude and height above sea level). (*However, Chemistry terminology is not always logical since a 'weighing bottle' should logically be termed a 'massing bottle').*
- In addition, no plurals, are added to SI names or unit, for example: 5 gram **not** 5 grams. This is, in part, to avoid confusion with the symbol s for seconds, but units do not have a plural form. Strictly speaking, all temperatures should be expressed as thermodynamic temperatures in kelvin. (Often expressed in the common but less correct absolute temperatures).
- However, unless gas law calculations are being performed, then temperatures are often expressed in degrees Celsius.
- The numerical value of a Celsius temperature expressed in degrees Celsius is given by: $t/°C = T/K - 273.15$ where t is the numerical value of a Celsius temperature and T is the absolute or thermodynamic temperature in kelvin.
- It follows that the degree Celsius is equal in magnitude to the kelvin, thus, temperature differences or intervals may be expressed in either the degree Celsius or the kelvin using the same numerical value.
- The specific heat capacity of water is approximately 4.18 J g^{-1} $°C^{-1}$ or 4.18 J g^{-1} K^{-1}.
- When using the unit of the mole a common mistake is to write, for example, 'number of moles of sodium chloride = 2.5 moles'. The correct approach is to write 'amount of sodium chloride = 2.5 mol'.
- Number of moles is a dimensionless number, e.g., 7, but amount is a physical quantity with an associated unit, e.g., 7 mol.
- Be careful not to use the word 'amount' in the everyday sense of the word where it is used in a much more wide ranging and 'loose' way and can refer to a number, a volume or even a weight. In the SI system the term 'amount' refers only to the mol.
- When referring to an amount (in mol) ensure that there is no ambiguity. Quote a formula or systematic name, for example, 1.0 mol of lead chloride might refer to lead(II) chloride, $PbCl_2$, or lead(IV) chloride, $PbCl_4$; 1.0 mol of oxygen might refer to 1.0 mol of oxygen atoms or 1.0 mol of oxygen molecules.
- The relative molecular mass is a dimensionless number, e.g., $M_r(H_2O) = 18.02$, *but* the molar mass is a physical quantity, e.g., $M(H_2O) = 18.02$ g mol^{-1}.

The term molecular mass should not be used to describe ionic substances such as sodium chloride, NaCl, since the lattice does not contain covalently bonded clusters of sodium and chlorine atoms. Instead, the lattice consists of a very large number of sodium and chloride ions (in a 1:1 ratio) each of which is bonded to several (theoretically all) other ions of opposite charge. The terms formula mass (g mol^{-1}) or molar mass (g mol^{-1}) should be used to describe ionic substances.

- When labelling graphs or tables with SI units, then the symbol of the unit is followed by a solidus(/), for example, V/ dm^3 and T/ K. This approach converts quantities to numbers by dividing the quantity by its unit.
- Note that the solidus notation is avoided within SI units, and scientific notation is preferred for example, mol dm^{-3} rather than mol/dm^3.
- A double solidus is forbidden, for example, is a/b/c meant to be (a/b)/c or a/(b/c)?

For example, the units of specific heat capacity should be written as J kg^{-1} K^{-1}. The equivalent expression using the solidus notation is J/(kg K), but its use is not encouraged. Another example is illustrated by a second order rate constant which has units of cubic decimetre per mole per second, which is expressed symbolically as dm^3 mol^{-1} s^{-1}, or dm^3/ (mol s) but not as dm^3/mol/s.

- Spaces, not commas, are used in numbers greater than 1000, for example, 101 325 Pa and not 101,325 Pa.
- All units in calculations should be expressed in SI base units (or units derived from them), for example, an energy calculation should give an initial answer in joules, which can then be expressed in kilo joules (kJ) (a multiple SI unit).

Always make sure that terms on either side of an equal sign are capable of being equal, for example, strictly speaking, you cannot write 100 °C = 373.15 K, just as 27 apples cannot equal 1.5 dollars. The correct approach to writing the above temperature conversion is: T/K = t/°C + 273.15. Therefore, T/K = 100 °C/°C + 273.15. Therefore, T = 373.15 K. However, many students (and IB Chemistry teachers) ignore this pedantry and simply write 100.00 °C = 373.15 K.

Non-SI Units

Several non-SI units may be encountered during your IB Chemistry programme. They may arise from the measuring device you are using or from data that you have obtained from the chemical literature. Ideally any raw data expressed in non-SI units (see *Figure 506*) should be converted to SI units before data processing.

Many non-SI units are now defined exactly in terms of SI units; some can only be related to SI units via fundamental constants and the relationship is therefore restricted by the precision to which the constants are known. Exact values are printed in bold type.

Non-SI unit	Unit type	SI conversion	Notes
Bar	Pressure	1 bar = 10^5 Pa	
Angstrom (Å)	Length	1Å = 10^{-10} m	Typical radius of an atom
Atomic mass unity (u)			Approximately equal to the mass of a proton or neutron; also known as a Dalton or amu
Minute (min)	Time	1 min = 60 s	
Hour (h)	Time	1 = 60 min = 3600 s	
Electronvolt (eV)	Energy	1 eV = 1.602×10^{-19} J	
Millimetre of mercury (mmHg or Torr)	Pressure	1 mmHg ≈ 133.322 Pa	
Atmosphere (atm)	Pressure	1 atm = 101.325 kPa	
Calorie (Cal)	Heat energy	4.184 Cal = 1 J	
Degree Celsius (°C)	Temperature	1 °C = 1 K	
Debye (D)	Dipole moment	3.336×10^{-30} C m	
Degree Fahrenheit (°F)	Temperature	5/9 K	
Curie	Radioactivity	3.7×10^{10} s^{-1}	

Figure 506 Non-SI units

Calculations with Units

Units should always be included during a chemical calculation. The advantages of using units throughout a calculation include an awareness that mathematical equations are not merely symbols, but express relationships between physical quantities; an in-built check on whether the correct equation has been used.

The following rules should be applied when performing arithmetic with units:

- Addition and subtraction: the units do not change

For example, 2.0 g + 5.0 g = 7.0 g

- Multiplication and division: the units multiply and divide too

For example, 3.0 cm × 3.0 cm = 9.0 cm^2; 10 kg × 9.8 m s^{-2} = 98 kg m s^{-2}

As a consequence, the units may cancel.

For example, $\frac{5.0\ g}{10.0\ g} = 0.5$

This worked example illustrates how the SI units of the ideal gas constant, *R*, may be deduced.

PV = *nRT*, rearranging, $R = \frac{pV}{nT}$

Substituting the SI units for each quantity gives:

$$R = \frac{Pa \times m^3}{mol \times K}$$

The units can now be 'multiplied out' as if they were just ordinary numbers. Pascals are pressure units representing the force (in newtons) on an area (in square metres).

The top line of the expression is thus N m^{-2} × m^3 = N m

(since powers are added when multiplying and subtracted when multiplying – the laws of indices)

But N m = J and the units can now be simplified to:

$$\frac{N\ m}{mol \times K} = \frac{J}{mol\ K} = J\ mol^{-1}\ K^{-1}$$

The laws of indices may need to be applied when dealing with equations containing derived SI units.

Two worked examples are shown below for equilibrium constants, K_c, which vary according to the equilibrium expression.

$$K_c = \frac{[H_2O\ (g)]\ [CO\ (g)]}{[H_2\ (g)]\ [CO_2\ (g)]} = \frac{(mol\ dm^{-3}) \times (mol\ dm^{-3})}{(mol\ dm^{-3}) \times (mol\ dm^{-3})}$$

The units on the top (numerator) and bottom (denominator) of the fraction cancel and K_c is unit-less or dimensionless.

$$K_c = \frac{[NH_3\ (g)]^2}{[N_2\ (g)]\ [H_2\ (g)]^3}$$

$$K_c = \frac{(mol\ dm^{-3})^2}{(mol\ dm^{-3}) \times (mol\ dm^{-3})^3} = \frac{(mol\ dm^{-3})^2}{(mol\ dm^{-3})^4} = \frac{1}{(mol\ dm^{-3})^2}$$

Simplify and then cancel any extra concentration units on the top (numerator) with those on the bottom (denominator), or vice versa:

$$K_c = = \frac{1}{(\text{mol dm}^{-3})^2} = \frac{1}{\text{mol}^2\ \text{dm}^{-6}} = \text{mol}^{-2}\ \text{dm}^6$$

Similar calculations can be performed to find the units for a rate constant. For example, consider a reaction with the rate equation: rate = k [A][B]^2

$$\text{mol dm}^{-3}\ \text{s}^{-1} = \text{k (mol dm}^{-3}) \times (\text{mol dm}^{-3})^2$$

$$\text{k} = \frac{\text{mol dm}^{-3}\ \text{s}^{-1}}{\text{mol dm}^{-3} \times (\text{mol}^2\ \text{dm}^{-3})^2}$$

$$\text{k} = \frac{\text{mol dm}^{-3}\ \text{s}^{-1}}{\text{mol dm}^{-3} \times \text{mol}^2\ \text{dm}^{-6}}$$

$$\text{k} = \frac{\text{s}^{-1}}{\text{mol}^2 \times \text{dm}^{-6}} = \text{dm}^6\ \text{mol}^{-2}\ \text{s}^{-1}$$

The following section contains a write-up of the planning part of an Investigation into a model lead-acid battery cell. It is *not* intended as practical work and it is *not* intended as a model write-up for an Individual Investigation, but it does describe how such an investigation could be presented and communicated. Relevant comments have been inserted at suitable locations and at the end. It is *not* a final write-up since no raw data has been collected, but it does show how the planning and trial phase of an Individual Investigation could be approached.

Investigating the Discharging and Charging of a model Lead-Acid Storage Cell

Research Question

The aim is to identify and investigate the effect that charge reversal, surface area of the lead electrodes and concentration of sulfuric acid have on the ability of a model lead–acid storage cell to hold its charge as measured by its ability to maintain a lit miniature bulb.

Introduction and Background information

A model lead-acid battery is constructed by immersing two lead plates in an aqueous solution of sulfuric acid.

The battery is then 'formed' by an initial charging using a power pack that causes the lead(II) oxide on the surface of one electrode to be reduced, while the lead(II) oxide on the surface of the other electrode is oxidised.

The relevant half equations describing the forming process are:

$PbO\ (s) + 2H^+\ (aq) + 2e^- \rightarrow Pb\ (s) + H_2O\ (l)$

$PbO\ (s) + 2H_2O\ (l) \rightarrow PbO_2\ (s) + 2H^+\ (aq) + 2e^-$

The relevant half equations and standard electrode potentials for the discharging process are:

$PbO_2\ (s) + 4H^+\ (aq) + 2e^- + SO_4^{2-}\ (aq) \rightarrow PbSO_4\ (s) + 2H_2O\ (l);\ E^\theta = 1.685\ V$

$Pb(s) + SO_4^{2-}\ (aq) \rightarrow PbSO_4\ (s) + 2e^-;\ E^\theta = 0.356\ V$

The overall cell voltage is thus 2.04 V under standard thermodynamic conditions and the overall equation for the discharging process is:

$PbO_2\ (s) + 4H^+\ (aq) + Pb\ (s) + 2SO_4^{2-}\ (aq) \rightarrow 2PbSO_4\ (s) + 2H_2O\ (l)$

$E^\theta_{cell} = 2.04\ V$

The capacity of the lead-acid battery is determined by the quantity of active materials present on its lead electrode surfaces. The capacity is proportional to the number of electrons that can be obtained from the surface and is measured in units of Ampere hours (Ah) for a commercial lead-acid battery.

It would be very helpful to include a discussion about a typical lead-acid battery from a car. Including a labelled cross-sectional diagram. Some background discussion about electrode potentials and standard conditions would also be helpful.

Personal motivation

I have a strong interest in electrochemistry following my construction of potato and fruit powered batteries during my Group 4 project. I am also familiar with the principles of redox chemistry. I have therefore decided to construct a model lead-acid cell and investigate its electrochemical behaviour. I have helped my Father maintain the lead-acid battery in his car and help check it (under his supervision) with a hydrometer, though now I note a trend toward sealed batteries.

This is a very helpful inclusion which can be used by the teacher to assess personal engagement.

Equipment used

aqueous sulfuric acid (4.00 mol dm^{-3})

sand paper

250 cm^3 glass beakers

lead foil (0.050 mm and 96.0 % purity) and scissors

electrical leads, wires and power pack (0 to 12 V)

safety glasses and sodium hydrogencarbonate/bicarbonate

miniature light bulb (2 V)

hammer and small nails

electronic stopwatch (precision ±0.005 s)

commercial water bath

Risk Assessment

Lead salts are toxic. Gloves and safety glasses are to be worn at all times. Lead salt residues will be stored in the heavy metals residues bottle. A supply of sodium hydrogencarbonate is to be retained to neutralise any acid spills. Residual sulfuric acid is to be neutralised with sodium hydrogen carbonate before being flushed down the sink with copious amounts of water. Voltages in order of excess of 6 volts are to be avoided in case of production of flammable mixtures of hydrogen and oxygen gases from the electrolysis of water (an expected significant side reaction). It is important that the electrodes are completely immersed: if the electrolyte is below the plate level, then an area of the plate will not be electrochemically efficient; this will cause a concentration of heat in other parts of the battery.

Classification of variables

Identification of dependent variable

The time for which test bulb remains lit.

Identification of independent variables

Variables that may affect the ability of the lead-acid storage cell to hold a charge include:

1. concentration of the sulfuric acid
2. temperature of the acid
3. surface area of the lead electrodes
4. time of the charging process
5. voltage used during the charging process
6. charge reversal during the charging process

The three independent variables chosen for investigation will be charge reversal, surface area of the lead electrodes and the concentration of sulfuric acid.

The predicted relationship between the lead-acid battery's capacity and the chosen variables is discussed next.

Charge Reversal

Charge reversals involve reversing the charging current by periodically switching the leads of the power pack during the charging process. The testing of this variable was prompted by the recent development of lead-acid batteries that can be rapidly charged by a pulsed current.

It is predicted that the amount of active material may be increased due to the action of the cycles of reduction/oxidation that roughen the surface of the lead electrodes thereby leading to an increase in their effective surface area.

It is expected that a small number of charge reversals will result in a measurable increase in the time the bulb remains lit. However, a large number of charge reversals are expected to have a smaller effect.

The following variables will be controlled during this investigation: concentration of the sulfuric acid, temperature of the acid, surface area of the lead electrodes, time of the charging process, and voltage used during the charging process.

Surface Area of the Electrodes

Research on the Internet and examination of Chemistry text books both reveal that commercial lead-acid batteries have grooved or perforated lead plates.

These references should be clearly stated and referenced.

The surface area of the electrodes can be increased by using a small hammer and nails to puncture the lead electrode surface with a series of small holes.

It is predicted that the amount of active material on the lead electrode surfaces will be increased in a directly proportional relationship as the surface area increases thereby leading to an increase in the ability of the battery to hold its charge.

The following variables will be controlled during this investigation: concentration of the sulfuric acid, temperature of the acid, charge reversals, time of the charging process, and voltage used during the charging process.

Concentration of Sulfuric Acid

The concentration of the sulfuric acid can be decreased by a dilution process.

The apparatus and approach for the dilution should be clearly described.

Considering the reaction for the overall cell discharge reaction as an equilibrium reaction:

$PbO_2\,(s) + 4H^+\,(aq) + Pb\,(s) + 2SO_4^{2-}\,(aq) \rightarrow PbSO_4\,(s) + 2H_2O\,(l) + PbSO_4\,(s);\ E^\theta = 2.04\ V$

All of the chemical species in this equilibrium, except the sulfuric acid and water are solids. If sulfuric acid (in the form of hydrogen and sulfate ions) was reduced in concentration in the lead-acid battery, then Le Chatelier's Principle would predict that the equilibrium would shift to the left, thus lowering the voltage. The Gibbs free energy change for the reaction will be minimised.

Planned Method

A 'trial and error' approach indicated that a safe and suitable charging process was 6 volts for a period of ten minutes using a pair of lead electrodes with dimensions of 1 cm × 6 cm.

Planned methodology

A lead-acid battery with fully immersed lead electrodes of dimensions of 1 cm × 6 cm is to be charged by 6 volts for a period of ten minutes in 4.00 mol dm^{-3} sulfuric acid (maintained at 25 °C). The capacity of the resulting cell is then to be measured by discharging it through a miniature light bulb (2 V) and recording the length of time it remained lit via the use of an electronic stopwatch.

The experiment will be repeated with 1 (once at 5 minutes), 2 (twice at 3.33 minutes and 6.66 minutes), 3 (three times at 2.5 minutes, 5.0 minutes and 7.5 minutes), 4 (four times at 2, 4, 6 and 8 minutes) and 5 charge reversals (with equi-intervals of 1.66 minutes), respectively. This is the dependent variable. The length of time the bulb remains lit is the independent variable.

Fresh sulfuric acid will be used for each experiment, but owing to the high cost of lead, the lead electrodes will be cleaned with fine sand paper and reused.

Any changes that occur in the sulfuric acid and on the surface of the lead electrodes will be recorded.

Time permitting, each of the charge reversal tests will be replicated three times and the average times calculated.

All other variables will be kept constant, namely: temperature of the acid (25 °C), surface area of the lead electrodes (6 cm^2), time of the charging process (10 minutes), voltage (6 V) used during the charging process.

Additional Author Comments

The investigation has a clearly defined research question and focussed problem as indicated in the title and aim. Three relevant variables have been selected. It might be preferable to have one research question and investigate one relevant variable.

Three separate testable hypotheses have been formulated that relate directly to the investigation. However, two of them are only qualitative – they predict the effect on the charging capacity, either a decrease or increase, but do not make quantitative predictions. The Nernst equation should be used to be quantify the effect of temperature and concentration on the voltage of the lead-acid cell. This is a missed opportunity.

(Strictly speaking, the major sulfate species present in battery acid is the hydrogensulfate ion, HSO_4^-. However, the equations given are adequate for IB Chemistry).

The various relevant variables that may affect the lead-acid storage cell's capacity are all identified. The predicted effect of changing three of them is briefly discussed with reference to electrochemical and equilibria concepts. Explicit details are given outlining how the three variables will be controlled and changed, as relevant.

The planning for investigating the effect of one of them, namely charge reversal on the cell's capacity, is outlined. The distance between the two electrodes and their thickness and purity, should be specified.

Appropriate materials and apparatus have been chosen and some preliminary experimentation work has been performed to establish a suitable and safe charging process.

A suitable method that allows the control of the variable, the number of charge reversals, has been given. Such an approach should allow for the repeated collection of relevant, reliable and sufficient raw data, namely discharge times.

Listed in Figure 507 is a summary of what you need to do to score well in the Communication criterion.

Assessment criteria	Evidence required	What you must do
Writes a well structured and clear report (write-up)	Structured report	The report must be well structured into different clearly designated sections and the English must be clear, correct and accessible. It should resemble the form of a scientific paper but must present relevant information on focus (the Research Question and introduction), process (the methodology) and outcomes (results and evaluation) in a coherent manner.
	Relevant and concise report with correct conventions and referencing	The report must be relevant and concise (10 pages). It should not contain irrelevant or tangential issues (those not directly relevant to your Research Question). The data collected should be relevant to the Research Question and support a justified conclusion. Subject Specific terminology (chemical terms) and conventions, for example, referencing and labelling of all data tables, graphs and digital images, or the use of the passive voice, should be appropriate and correct. Data should be processed and displayed with the correct type of graph. All literature consulted should be referenced and cited according to well known conventions. Any errors in the report should be minor and not hamper understanding of the investigation.
	Units and calculations	Calculations should be accompanied by appropriate units, usually SI. Calculations should be carried out according to the rules of significant rules and final values reported to the correct number of significant figures. Error propagation should be performed and the working shown in the report. It may also be appropriate to show how the final units of a calculation are derived. Some simple statistics may be relevant.

Figure 507 Summary of the Communication criterion

The information in the following table provides some indication of how the Extended Essay will be assessed. Individual teachers and schools may provide additional information as they wish.

Assessment criterion	Highest mark for criterion	Description of highest achievement level for each criterion.
A: Research question	2	The research question is clearly stated in the introduction and sharply focused, making effective treatment possible within the word limit
B: introduction	2	The context of the research question is clearly demonstrated. The introduction clearly explains the significance of the topic and why it is worthy of investigation.
C: Investigation	4	An imaginative range of appropriate sources has been consulted, or data has been gathered, and relevant material has been carefully selected. The investigation has been well planned.
D: Knowledge and understanding of the topic studied	4	The essay demonstrates a very good knowledge and understanding of the topic studied. Where appropriate, the essay clearly and precisely locates the investigation in an academic context.
E: Reasoned argument	4	Ideas are presented clearly and in a logical and coherent manner. The essay succeeds in developing a reasoned and convincing argument in relation to the research question
F: Application of analytical and evaluate skills appropriate to the project.	4	The essay shows effective and sophisticated application of appropriate analytical and evaluative skills.
G: Use of language appropriate to the subject	4	The language used communicates clearly and precisely. Terminology appropriate to the subject is used accurately, with skill and understanding.
H: Conclusion	2	An effective conclusion is clearly stated; it is relevant to the research question and consistent with the evidence presented in the essay. It should include unresolved questions where appropriate to the subject concerned.
I: Formal presentation	4	The formal presentation is excellent
J: Abstract	2	The abstract clearly states all the elements listed above. The requirements for the abstract are for it to state clearly the research question that was investigated, how the investigation was undertaken and the conclusion(s) of the essay.
K: Holistic judgement	4	The essay shows considerable evidence of such qualities (qualities that distinguish an essay from the average, such as intellectual initiative, depth of understanding and insight). © IBO 2014

The Extended Essay in Chemistry

The Extended Essay is one of the core requirements of the IB Diploma Programme. The Extended Essay is an academic study of a focused chemical research question. It is intended to give you the experience of working on a research project under the guidance of a chemistry teacher who acts as your supervisor. They will meet with you a number of times and comment on the final draft of your Extended Essay. He or she may also conduct a short interview, known as a *viva voce*, after your Extended Essay (maximum of 4000 words) is complete. The Extended Essay is graded on a scale from A (highest) to E (lowest).

Extended Essays in chemistry may involve the following broad research areas: energetics, kinetics, stoichiometry, organic chemistry, transition metal chemistry, main group chemistry, solid-state chemistry, reaction kinetics (for example, catalysis), food chemistry, stereochemistry, polymer chemistry, electrochemistry, chemical and physical equilibria, thermodynamics, chemical bonding and intermolecular forces.

The scope of the project is open-ended and the topic or phenomenon and associated theory under study may not necessarily appear in the IB chemistry syllabus, for example, a study of an oscillating chemical reaction, the formation of azo dyes by diazo coupling reactions or the formation of Liesegang rings (in a gel).

The Extended Essay may involve the collection and analysis of primary data from the published literature. However, the majority of Extended Essays also involve the collection and analysis of primary data often using relatively simple apparatus or techniques. In other words, you carry out investigations in the chemical laboratory and collect raw chemical data, but you should also consult primary data from the chemical literature.

The most successful Extended Essays in chemistry are those based on a small number of a clearly defined and easily manipulated independent variables and a single quantifiable and easily measured dependent variable.

It should be noted, however, that it is the approach to the Extended Essay rather than the topic itself which will determine whether the investigation is suitable to be developed into an Extended Essay. For example, the reaction of magnesium with dilute acids can, for example, be treated in a very superficial manner in which only the effect of acid concentration on rate of reaction is explored.

The same topic can also be investigated to a much deeper approach where the effect of different acids (strong, weak and oxidizing, such as nitric(V) acid) are compared, the effect of temperature is considered and the effect of added cations and anions on the interactions taking place at the magnesium surface are investigated. An Extended Essay should only investigate one of these variables in depth.

It is important to have a clear and sharply focused Research Question to guide your Extended Essay. This should be generated by you in discussion with your supervisor.

Below is an outline of a chemistry project plan in the context of an Extended Essay. Suitable critical comments have been added.

Research Question

Is there a relationship between the equilibrium constant (K_c) and temperature for the reaction of hydrogen and iodine (in the gas phase)?

You will then need to formulate an Aim perhaps with a testable and chemically justified hypothesis.

You must also justify the worthiness and significance of the Research Question – this has not been done here. Some reference to the industrial synthesis of hydrogen iodide may be helpful.

A hypothesis should be testable and falsifiable which means that your results should either support the hypothesis or show it to be false. However, the inclusion of a hypothesis is not a requirement of the assessment criteria and may only be appropriate for certain topics or areas of chemistry.

(N.B. possible teacher comments are shown in red)

Aim

To find values of K_C (equilibrium constant) over a range of temperatures for the equilibrium:

$H_2\,(g) + I_2\,(g) \rightleftharpoons 2\,HI\,(g)$

Hypothesis

If ln K_C is plotted against $1/T$, the slope of the curve at any point is equal to $-\Delta H_\theta/c \times R^{-1}$ (c is a unit conversion constant: R is the gas constant). If ΔH^θ is constant over a range of temperatures then this should produce a straight line graph.

This chemical background needs further explanation and justification from thermodynamics.

You will need to be identify what data you plan to obtain and outline a procedure to obtain the raw data and process it.

Data to Obtain

Concentrations of iodine and hydrogen iodide in the equilibrium mixture for at least 5 different temperatures. Temperatures are to be converted to the absolute or thermodynamic scale of temperature (Kelvin). Concentrations to be measured using titration, concentrations are converted into K_c using the following equilibrium expression:

$$K_c = \frac{[HI(g)]^2}{[H_2(g)][I_2(g)]}$$

Procedure

Equal quantities (in moles) of hydrogen and iodine will be placed in a thick walled glass flask and allowed to reach equilibrium at constant temperature. The temperature will vary between 400 and 500°C at 20°C intervals using an electric furnace. Each experiment will be repeated, at least once.

The student should discuss the various options that were open to them, why they chose the one(s) they did and ways in which they found they needed to modify it as a result of initial trials.

It will be assumed that the equilibrium has been reached by visual inspection for the intensity of the iodine colour (the use of a uv-vis spectrometer will also be investigated). Once equilibrium has been reached the mixture will be rapidly quenched in an accurately measured volume of cold potassium iodide solution where both the iodine and the hydrogen iodide will readily dissolve. Samples of this reaction mixture will be titrated separately against aqueous sodium thiosulfate (to measure the iodine) and freshly prepared aqueous sodium hydroxide (to measure the hydrogen iodide).

Equilibrium concentrations of these components will be measured by titration, and the hydrogen concentration calculated by difference. Each titration will be repeated twice.

The student should explain why they chose this method rather than just measuring one of these and the initial amount of one of the reactants.

Once your supervisor has discussed safety issues then you may be allowed to start preliminary data collection. You may then need to modify your method and/or the concentrations of chemicals. You may also be required to carry out a risk assessment before any practical work is allowed to commence.

All science Extended Essays are marked according to the same assessment criteria and to gain high marks you must address these assessment criteria fully and completely. You must not present your Extended Essay in the same way that you present your Individual Investigation. It should not be written as a laboratory report. There are eleven separate criteria worth a total of 36 marks.

Criterion A: The Research Question

A focused Research Question is the first step in a successful Extended Essay in chemistry and should be stated in the introduction preferably (in bold), perhaps at the end of the introduction. It must be clearly focused on chemical principles, and capable of being answered within the word limit and a reasonable time frame (a suggested 40 hours) of an Extended Essay. You may need some assistance from your supervisor to help formulate a research question from a topic you are interested in. You should not have several dependent variables leading to two ore more Research Questions since they may indicate a lack of clear focus.

The Research Question does not have to be a question; it could be a statement which outlines what you are trying to discover. A Research Question clearly states the variables that are to be manipulated, measured and analysed.

An example of a Research Question related to an oscillating reaction:

To investigate the effect of temperature on the period of oscillations in the Briggs Rauscher reaction.

An example of a Research Question from analytical chemistry:

What factors affect the accuracy of the colorimetric determination of the nickel content in steel?

An example of a Research Question from physical chemistry:

Determining the partition coefficient for several dicarboxylic acids with water and 2-methylpropan-1-ol and interpreting the results in terms of intermolecular bonding.

Research Questions can come from a number of different sources. They may be formulated after carrying out an investigation (as part of your Internal Assessment) or watching a teacher's demonstration. They may be reactions you have viewed on the Internet or described in your text book.

The Research Question must appear on the title page, abstract and in the introduction. The Research Question must be identical in all the places where it occurs in your Extended Essay. The Research Question may or not be the title of the Extended Essay.

The Research Question should allow you to apply your knowledge of IB chemistry and analysis of data in a personal way. You should not choose a Research Question that is an extension of your Internal Assessment (IA) or can be easily answered by looking at an IB chemistry text book.

Try and avoid topics that are frequently addressed by other candidates, such as those involving vitamin C, aspirin and caffeine. Also avoid non-quantifiable independent variables, such as 'Comparing the percentage of acetylsalicylic acid in different brands of aspirin tablets'.

There are a number of publications that can be sources of ideas or topics for investigation by a chemistry Extended Essay: School Science Review (*Figure 601*) <*http://www.ase.org.uk/journals/school-science-review*> published by the Association for Science Education (ASE), Chemistry Review published by Philip Allan <*http://magazines.philipallan.co.uk/Holding-Page1.html*>. The Journal of Chemical Education is another useful resource.

EBSCO <*http://www.ebscohost.com*> and Science Direct <*http://www.sciencedirect.com*> (produced by Elsevier) are on-line databases subscribed to by many International schools. Find put out from your Library Supervisor whether your school has access. There are also two CDs available from the on-line IB shop <*https://store.ibo.org/diploma-programme*>, called 50 Excellent Extended Essays, which contain useful exemplars, for supervisors and students.

Figure 601 Screenshot of the ASE web site

Criterion B: Introduction

The introduction should include relevant background to the study, which means any theoretical or previous experimental work or observations that led to the Research Question. Background information will include references to published work in books, papers from the chemical or educational literature and on-line web sites. It may also include a brief review of competing hypotheses or interpretations of data. You should also discuss any personal motivation and personal involvement you have in selecting your investigation worthy of at least 40 hours of work.

There are three aspects to this criterion: the chemical context, the chemical significance and the importance and significance of the investigation. In order to score the highest mark all three aspects must be addressed. In order to demonstrate the chemical context and significance and worthiness of the research question you need to present a summary of the literature (typically published papers and journal reviews) and other external sources, such as book chapters, that you have consulted. You should avoid making any sweeping statements with no attributable sources. Also avoid introducing advanced theory, that is only poorly understood and not used in the processing and analysis of the results.

For example, your Extended Essay may involve the study of the coordination reaction between copper(II) ions and aspirin. Aspirin is a widely used non-steroidal anti-inflammatory agent used for the treatment of inflammatory diseases, such as arthritis. However, its effectiveness is limited due to its low potency. In certain cases, the relief of pain and control of inflammation require large doses and such quantities can cause peptic ulcers and stomach bleeding.

Copper complexes involving anti-inflammatory drugs can be more effective at treating rheumatoid arthritis and involve less side effects than the free (uncomplexed) drug. You will need to discuss the nature of the coordinate bond and draw the structure of the complex. This can be done using Lewis theory and perhaps in terms of orbitals.

Criterion C: Investigation

This criterion covers both data collected from printed sources as well as data collected by the candidate (through doing experiments in the laboratory). You will be judged about the range, accuracy and appropriateness of the data you have collected as well as the method used to obtain the raw data. You must show strong evidence of planning and exploratory investigative work. You should explain how information from your sources (on-line and print) helped you decide on your approach. The relative merits and disadvantages of other methods should be discussed.

Your method must be reproducible and full details of all apparatus and instrumentation should be given including the random uncertainty (tolerance) and range, where appropriate. Any modifications to a well-known protocol, such as the Winkler method, or titrimetric method, such as a back titration with EDTA, should be outlined and justified. Do not describe unnecessary and trivial experimental details.

Criterion D: Knowledge and understanding of the topic studied

You can display knowledge and understanding of the topic by presenting relevant background information and explaining how this relates to the Research Question. You can demonstrate understanding by referring to the variables that may affect the investigation and by referring to the significance of the outcomes. You should provide explanations and justifications for your apparatus and methodology and choice of techniques to process, present and analyse your data. You should also explain why alternative approaches were considered but not adopted.

Equations from physical chemistry should be clearly explained. Symbols should be explained and appropriate units stated for physical quantities. Where possible and appropriate the equation should be derived or justified in an informal chemical sense. Any weaknesses or limitations in the law or relationship described by the equation should be outlined. For example, the Beer-Lambert law does not hold at high concentration and the relationship often becomes non-linear at absorbances greater than two. The Nernst equation only holds under standard thermodynamic conditions and only applies to a redox system at equilibrium. You should not simply present mathematical formulas and 'plug' in numbers without a clear understanding of the mathematical relationship of the variables involved.

You should demonstrate appropriate chemical and mathematical knowledge, such as the rules for significant figures. You should have a firm grasp of any physical and biochemical concepts relevant to your Extended Essay. You do not need to explain and justify simple chemical facts, principles or concepts from the core of the IB Chemistry programme.

Criterion E: Reasoned argument

A convincing argument in relation to your Research Question is key to the success of development of a well written Extended Essay. You should set out your ideas clearly and logically and analyse the strengths and weaknesses of your claims. You should not arrive at a conclusion to your experimental work without questioning any chemical assumptions or considering possible competing explanations (counter claims). You should attempt to analyse the validity and reliability of any secondary sources of data you have used. This is the criterion that often distinguishes excellent Extended Essays from the mediocre.

Criterion F: Application of analytical and evaluative skills

Criterion F requires you to apply appropriate chemical analytical and evaluative skills. This includes deductive reasoning (generalizing from examples), graphical analysis and mathematical analysis (where appropriate). You should also analyze the validity of your secondary resources, by careful reading and cross-referencing to test their reliability. There should be a thorough understanding of the data collected and the magnitude of systematic errors, limitations or random uncertainties of the experimental design.

Criterion G: Use of language

There are two aspects to this criterion: the use of clear and precise language and the use of terminology appropriate to the chemical topic.

For example, chemical names should not be capitalized (unless at the start of a sentence) and formulas should be used in equations and not in text.

IUPAC names, including Stock notation (involving oxidation numbers), should be used consistently in the Extended Essay, where appropriate, for example, potassium manganate(VII), and not potassium permangnate. If trivial names are used, such aalanine, then the IUPAC name (2-amino ethanoic acid) should be stated when it first occurs and equated to the trivial name. Any stereo-chemical prefixes should be used, where appropriate, for example, S-2-bromobutane and D-alpha-glucose. Where relevant, correct displayed structural formulas should be included.

You need to have a clear and precise style and show an understanding of and fluency in the main chemical terms associated with the topic.

For example, if your Extended Essay is concerned with investigating some aspect of kinetics then chemical terms and concepts, such as mechanism, order, rate determining step, etc. are likely to be present in the write-up. The more technical and unfamiliar terms, such as auto-catalysis and pseudo order should be defined before use, perhaps in the form of a glossary in the Appendix.

There is no requirement to write in the passive voice, for example, *the mixture of propan-2-ol and acidified potassium dichromate(VI) was refluxed for ten minutes at 60* ° C. You can use the first person singular, active voice, for example, *I refluxed the mixture of propan-2-ol and acidified potassium dichromate(VI) for ten minutes at 60* ° C. However, you must be formal, consistent and use key terms accurately.

Criterion H: Conclusion

In an effective conclusion, which must be consistent with the body of the essay, you should restate the research question and outline the extent to which it has been answered, dealing also with issues that have not been resolved and suggesting future research directions. You should refer to your quantitative outcomes (processed data) but must not overstate your findings and always be tentative in your conclusions. Use statements along the lines of the following: t*he graph suggests a possible relationship between variables X and Y.* Note that no new material should be presented at the conclusion.

Criterion I: Formal presentation

You should follow a well known format for correct referencing, for example, MLA (Modern Language Association). A table of contents must be included and the main body of the essay page-numbered. You should not use the appendix as a way of keeping the word count below 4000 words. New information should not be introduced into the Appendix since the Extended Essay examiner is not required to read these pages.

Examples of correct referencing:

Talbot, C. (1999) The Briggs Rauscher reaction. *School Science Review*, June 2012, 93 (345), 9-10.

Zutter, U. *et al.* (2008), New, efficient synthesis of oseltamivir phosphate (Tamiflu) via enzymatic desymmetrization of a meso-1,3-cyclohexanedicarboxylic acid diester. Date accessed: 12.9.14

<http://www.ncbi.nlm.nih.gov/pubmed/18517254>

Green, J., and Damji, S. (2014) Chemistry for the IB Diploma. *IBID Press*.

Criterion J: Abstract

Writing an abstract is a difficult requirement for many students. It is suggested you consult any reputable journal and examine abstracts from published chemical papers or Extended Essays provided by the IBO.

The writing of the abstract should be left after you have written the main body of the Extended Essay. It should not be part of the page-numbering.

An abstract should include the following in three separate paragraphs: the Research Question, an outline of the method including any controls, a summary of the data collected and its analysis), a discussion of important assumptions and errors, and the conclusion.

The abstract must match the research question and give sufficient details of how the investigation was undertaken. The abstract must not exceed 300 words.

The Appendix

Examiners of the Extended Essay are not required to read these, nor can they take them into account in the grade they award, so vital aspects should not be relegated to one. For example putting the 'procedure' as an Appendix would have a significant impact on the grade an Examiner could award.

7.1 Introduction

For ten hours of your IB Chemistry course you are required to participate in a Group 4 Project. The intention of the Group 4 project is that students from the Group 4 subjects: Sports, Exercise and Health Science, Chemistry, Physics, and Biology work together to investigate or solve a common problem. ESS (Environmental Systems and Studies) students are not mandated by the IBO to be involved in the group 4 project, though your school may have them participate. It is a compulsory component of the IB Diploma Programme and is usually completed in the first year of the IB Chemistry Programme.

This aim is to provide all students with the opportunity to appreciate both the implications of using science and the limitations of scientific study, in a local context. The main philosophy of the Group 4 Project is to emphasize interdisciplinary co-operation and the processes involved in a scientific investigation rather than the products of such an investigation.

The IBO also encourages collaboration and cooperation between schools for the Group 4 Project. Students are expected to conduct ethical experiments which are aligned with the IBO's animal experimental policy and Ethical practice poster. The IBO also allows theoretically based investigations, such as spreadsheet modeling, use of on-line databases or analysis of secondary data.

Schools differ in the arrangements they make for the Group 4 project but essentially it is separated into three distinct phases: planning, action and evaluation. *Figure 701* shows some ideas for a Group 4 project that takes place in a swimming pool and the theme of keeping cool.

7.2 Planning

This takes about two hours. You will meet either as a whole IB group or cohort and then probably in smaller mixed groups if you are a student in a school with a large number of IB students. Ideally the students in your school will have a 'brainstorming' session and agree on an overall topic, for example, the school canteen, acid rain or the school swimming pool or theme, for example, water, energy or light. The topic may be related to either the school itself or the local area. Once the overall topic is agreed then either individually or in small groups you will plan your own particular contribution to the chosen topic. At this stage you will need to plan what equipment, and chemicals you will need, prepare a plan of action and submit a risk assessment. If you are liaising with other IB schools you will want to inform them of your plans at this stage.

7.3 Action

About six hours is devoted to the action stage. You can investigate your topic or theme either in mixed subject groups or in a chemistry group. Some schools spread this time out over one or two weeks others complete it in a day or weekend. Remember the aim is on the process not the product, in other words, you might not obtain reliable results or they may not prove amenable to analysis. You may plan to do experimental work but it is perfectly permissible and sometimes more efficient to get your data from elsewhere. For example many chemistry contributions to the Group 4 project involve the analysis of samples of freshwater water. Some simple practical analysis, for example, redox titrations can be performed using the facilities of a normal school laboratory. However, by contacting a local water provider you might be able to obtain a much more accurate and sophisticated analysis of your local water. If you do perform your own practical work then you must pay attention to safety, ethical and environmental considerations.

If you are studying two science subjects for your IB Diploma then you do not need to carry out the action stage of the Group 4 Project twice.

7.4 Evaluation

The time allotted to this is usually about two hours. The emphasis during this stage is on sharing your findings, both successes and failures, with other IB Diploma students. There are many ways in which you might do this. Some schools devote a morning, afternoon or evening to a symposium where all students, as individuals or as groups, give brief presentations, perhaps involving Power point presentations and/or videos. Your school may invite parents. Others take the form of a science fair where students circulate around posters summarizing the results of each group or all the students in the school could contribute their findings to a specially designed webpage on the school's Intranet or the OCC (On-line Curriculum Centre).

Topic/theme/context	Chemistry	Physics	Biology
School swimming pool	Determination of chlorine content via redox titration; study of the decomposition of chlorine water in the presence of sunlight; study of chemicals used to chlorinate pool water; relationship between free chlorine and pH; effect of urine in pool water	Determination of physical properties of chlorinated water, e.g., density, specific heat capacity, refractive index; surface tension, boiling point, melting point; change in pressure with depth, heat loss due to evaporation; measurement of heat gain during day, heat loss at night	Culturing of bacteria, algae (effect of pH) and fungi; effect of changes in chloric(I) acid concentration and pH on microorganism growth; pathogens present in polluted pool water from faeces; the diver's 'bends'
Keeping cool	Determination of the amount of sodium chloride and urea in sweat; investigation of the reactions in cool packs. Study of chemicals used in air conditioners: CFC, HFC, impact on global warming	Investigating the ability of different surfaces and colours in reflecting solar energy; studying the design and effectiveness of a cool box, air conditioner and thermos flask.	Investigation of the changes that occur in the souring of milk or red wine; measuring the transpiration rate under different environmental conditions

Figure 701 Some ideas for Group 4 Projects

Exercise

Imagine you are going to visit a mangrove swamp (*Figure 702*) to carry out a Group 4 Project.

Generate some possible investigations for Chemistry, Physics, Biology and Sports, Exercise and Health Science.

Figure 702 Mangrove swamp in Northern Singapore

7.5 Self motivation

Listed below are some ways by which you can demonstrate your self motivation and perseverance.

7.5.1 Planning Stage

- arriving to meetings or brainstorming sessions on time.
- coming to meetings or brainstorming sessions prepared. Once you have discovered the general theme of your Group 4 project you are expected to conduct some research about the topic.
- contributing positively to the brainstorming session. Be supportive of ideas.
- staying focused during the meeting. When you are not speaking, be an active listener. Take down notes if you hear something important.
- submitting the planning sheet on time (if applicable).

7.5.2 Action Stage

- Ensuring that the apparatus chosen and methodology for the project will give precise and reliable results.
- Presenting a creative approach to the problem.
- Making sure that you know and understand the methodology to be performed during the investigation. This includes being able to identify the data to be collected and how these data are to be collected.
- Finding and suggesting ways to solve the problem if the team is encountering difficulties with the project.
- Adapting to new circumstances. If an unexpected result is obtained, then you must try to make sense of this result or perform additional measurements to verify the reliability of this result.

7.5.3 Evaluation

- Approaching the Project with integrity. This includes acknowledging resources that were used and not altering the data to fit a preconceived **hypothesis**.
- Presenting or contributing positively towards an effective method to present your findings, successes and failures to other teams.
- Being available to other teams to help them better understand your Group 4 Project.

7.6 Working within a team

A good team will work more effectively than individuals.

7.6.1 Planning Stage

During the Planning Stage of the Group 4 Project, your ability to work with a team can be demonstrated by:

- Arriving to the meetings and planning sessions on time. This suggests that you value the time of your team mates.
- Responding to a different idea in a supportive fashion. Look at the strength of the idea first before stating its perceived weaknesses. This shows you value your team mates' ideas and this can encourage further exchange of ideas.
- Readily sharing ideas and asking questions.
- Listening to and not interrupting the speaker.
- Accepting and following the collective decision of the team even if you do not agree with it.
- Taking the initiative to contact other members of the team to update yourself should you miss a planning session.

7.6.2 Action stage

During the Action Stage of the Group 4 Project, your ability to work with a team can be demonstrated by:

- Leading by example.
- Completing the task assigned to you to the best of your ability and, if necessary, seeking assistance from other members of the team.
- Readily assisting other members of the team to the best of your ability.
- Acting responsibly and not performing any action that will place the other members of the team or the other teams in unnecessary danger. This includes seeking assistance from your IB teacher in matters involving a breach of safety.

Due to some personal differences, it possible that your team or a few members of the team do not work well together. This will prevent your team from completing the Group 4 project well. It is suggested that you take time to discuss the problem as a team. During the discussion, it is important that the team stick to the issues and avoid personal attacks. Everyone should be courteous, respectful of other people's opinions, and open to other people's ideas. If a problem concerns one or two individuals only, then someone can act as a moderator and discuss the issues privately with this individual(s).

As much as possible, the team must resolve the issues amongst themselves quickly. Discussing the problem with your IB teacher should be the last resort. Also, requesting to be transferred to another group suggests poor collaborative skills on your part.

7.6.3 Evaluation Stage

During the Evaluation stage of the Group 4 Project, your ability to work with a team can be demonstrated by:

- recognizing the strengths of the team and of the individual members of the team. This can be done by contributing positively to the presentation of the team's successes.
- Suggesting ways and methods by which the weaknesses of the team is eliminated or reduced. This includes proposing ways which will prevent the same mistakes being committed again.

7.7 Self-reflection

You might be asked to reflect and write a self evaluation report. If this is the case, below are suggested questions that can help you conduct a thorough self-reflection.

7.7.1 Planning Stage

- Did you contribute positively towards the planning of the investigation? If yes, what preparations did you do? Could you have contributed more? What prevented you from doing so? How can you overcome these obstacles?
- If you did not contribute positively, what prevented you from doing so? How can you overcome these obstacles next time?
- Were you able to accept differing ideas easily? Did you attempt to look at both the strengths and weaknesses of a proposal? Did you analyse the proposal objectively? If not, what prevented you from doing so? How can you overcome these obstacles?

7.7.2 Action stage

- Did you have the necessary skills to conduct the investigation efficiently and safely? Which skills were you good at? Which skills do you need to improve on? What do you need to do to improve these skills?
- Did your actions help promote effective collaboration amongst the different members of the team? What could you have done better for the team to improve collaboration amongst the members?
- What went well for the team? Why did the team encounter such difficulties? What could you have done better for the team to help it complete the investigation effectively?
- Did you help the team manage the time effectively?

7.7.3 Evaluation

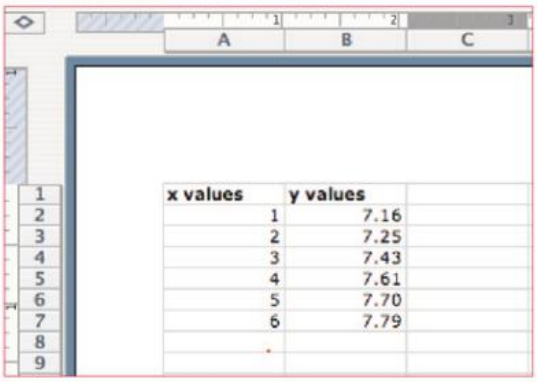
- What insight(s) did you gain from the conclusions obtained?
- Was the team able to present its findings accurately and clearly? If yes, how was team able to do it? If not, what prevented the team from doing so?
- Did you contribute positively towards the team's presentation? What could you have done better to help the team present its findings more accurately and clearly?

8.1 Spreadsheets

A spreadsheet is the most commonly available software application suitable for analyzing and displaying of data. The data may be added manually via the keyboard or imported from files. One of the most important uses of a spreadsheet is that it allows its data to be analysed graphically. Two or more sets of corresponding data can be plotted as histograms or as simple scatter graphs.

Using Excel to Present Processed Data

The tutorial below with associated screenshots show how to plot a line graph with error bars and perform a least squares regression analysis using Excel. The least squares approach allows you to draw a line of best fit through experimental data. On the spreadsheet enter the name of your x–variable into cell A1 and the name of your y–variable into cell B1. Enter your x–values into the remaining cells of column A and the corresponding y–values into column B (*See Figure 801*).



	A	B	C
1	x values	y values	
2	1	7.16	
3	2	7.25	
4	3	7.43	
5	4	7.61	
6	5	7.70	
7	6	7.79	
8			
9			

Figure 801 Six pairs of x and y values in Excel

Highlight both columns of numbers with the mouse. From the Insert menu, select Chart. In the first window of the Chart Wizard, select XY(Scatter) as your chart type, and compares pairs of values (the first box in the first column) as your chart sub-type. Click on Next. In the second window of the Chart Wizard, in the Data Range screen, ensure the series in Columns is selected and then click on Next. In the third window of the Chart Wizard, type in a suitable title for your graph. Type in labels for your x and y axes, and remember to include units using the solidus notation. It may be helpful to click on major x and y gridlines. Click on Next. In the fourth window of the Chart Wizard, select As New Sheet. Click on Finish. A graph should appear on a new sheet in your work book.

To perform least squares analysis click on the line itself so that the points of the line become highlighted. Pull down the Chart menu and select Add Trendline. In the Type window, select Linear as your trend/regression type. Click on the Options tab at the top of the window, and select Display equation on chart and Display r-squared value on chart in the Options window. Click on OK. A straight line and an equation in the form and a value should appear (*Figure 802*) '*r*' is the correlation coefficient of your least squares determined line. The closer is to 1, the better the fit of your data points to a straight line.

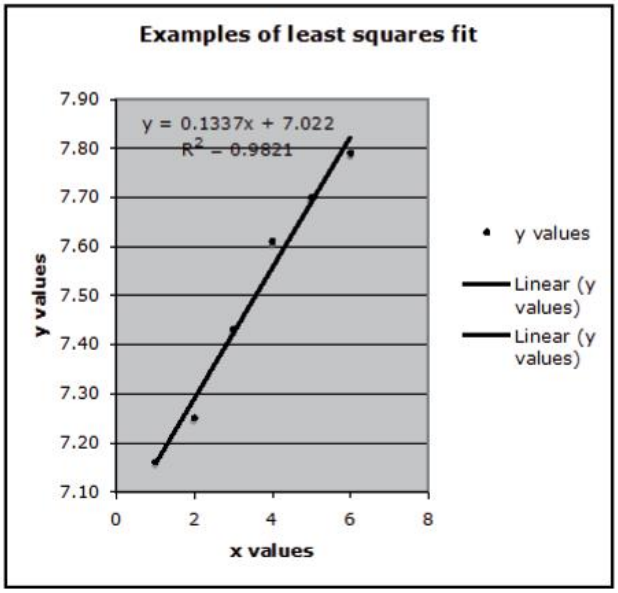


Figure 802 An example of an Excel generated least squares fit

Plotting a Graph with Error Bars using Excel

To plot a graph with error bars follow these steps: Enter the data and highlight both columns with the mouse. From the Insert menu, select Chart … In the first window of the Chart Wizard, select XY(Scatter) as your chart type, and data points not connected by lines (the first box in the first column) as your chart sub-type. Click on Next. To add the error bars, highlight all the data points by clicking. From the Format menu, click Selected data series and then select the Y error bars tab and enter the appropriate value for the uncertainty.

Constructing an Arrhenius Plot using Excel

We will calculate the activation energy and rate constant at 37 °C from an Arrhenius plot of the data in *Figure 803*:

Temperature/ °C	Rate constant, k/s^{-1}
24	4.8×10^{-3}
28	7.8×10^{-3}
32	1.3×10^{-2}
36	2.0×10^{-2}
40	3.2×10^{-2}

Figure 803 Kinetic data for an Arrhenius plot

The data is typed into Excel. Cells A1 and B1 are used as the headings. Cells A2–A6 are the temperatures in degrees kelvin and B2–B6 are the rate constants, *k*. The equation to calculate the inverse of the absolute temperature is typed in cell C2 (=1/(cell)). Upon entering Return, the value is displayed. The cell C2 result is highlighted and the corner of the cell dragged down to tabulate the rest of the values. The corner of cell C2 is dragged down to C6 and the pointer is released. The resulting values are tabulated for cells C3 to C6. The equation (=LN(number)) to calculate the natural logarithm of the rate constant, *k*, is entered in cell D2. The resulting values for cells D2 to D6 are then tabulated.

The values in cells C2–C6 and D2–D6 are highlighted and the Chart Wizard is selected to plot a graph. The scale can be adjusted by clicking on the y axis: Format Axis options appears. Select Scale and set the maximum value to –3 so the graph is maximised to this data point. The data points are highlighted. The Chart menu is selected and the Add Trend Line option is selected. The Option menu is selected and the Display equation on chart and Display r-squared value on chart are selected. Refer to *Figure 804*.

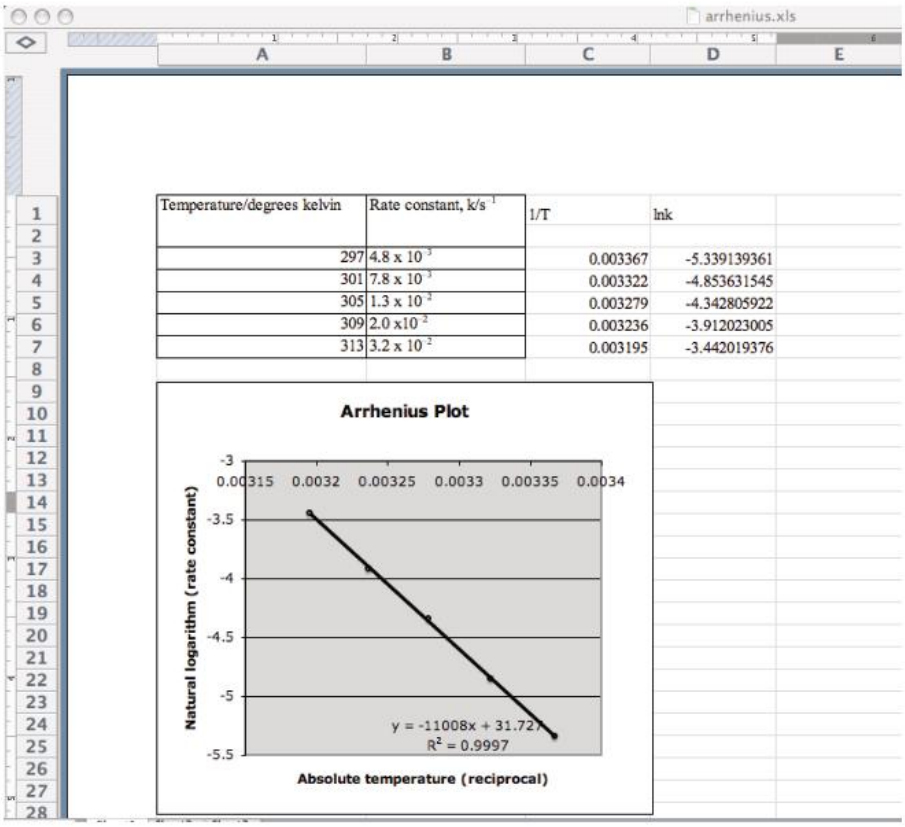


Figure 804 Arrhenius plot

From the equation of the line: $y = -11008x + 31.727$ the following information is determined:

1. From the y intercept we have that ln $A = 31.727$.

So that $A = e^{31.727} = 6.0098 \times 10^{13}\ s^{-1} = 6.01 \times 10^{13}\ s^{-1}$

2. From the slope: $m = -11008$ which equals $-\frac{E_a}{R}$.

Multiplying –11008 by $-R$ (-8.314 J K^{-1} mol^{-1}) yields

$E_a = 91520.5\ J\ mol^{-1} = 91.5\ kJ\ mol^{-1}$

The activation energy (E_a = 91520.5 J mol^{-1}) together with the natural logarithm of the pre-exponential value ($A = 6.0098 \times 10^{13}$) is now used in the exponential form of the Arrhenius equation: $k = A \times e^{\left(\frac{E_a}{RT}\right)}$, where T = 310 K.

So, $k = 6.0098 \times 10^{13} \times e^{\left(\frac{91520.5}{8.314 \times 310}\right)} = 0.023\ s^{-1}$.

Spreadsheets can also be used to help you investigate graphically the effects of concentration of reactants on the rate of reaction. Simple modelling of chemical systems, for example, of chemical equilibrium or acid-base titration curves, can be carried out using the spreadsheet. You can explore 'what-if' situations in such cases.

Simple modeling of enthalpy changes with Excel

The enthalpy change of combustion can be easily calculated from bond energies. The energy needed to break all the bonds in the reactants are summed and added to the energy needed to form all the bonds in the products. Bond breaking is endothermic and bond formation is exothermic. The enthalpy change is calculated by summing together the values with their associated signs.

The Excel spreadsheet in *Figure 605* calculates the enthalpy change of combustion of methane. All the text: title, headings and bonds are typed into the cells. Each cell in the spreadsheet has a cell reference, for example, cell A3 contains Compound; Cell B7 contains 348. All bond energies are taken from the IB Data Booklet.

Some of the cells contain formulas needed to perform the calculation. For example, B9*C9 is instructing Excel to multiply the entry in B9 the bond enthalpy of the C-H bond) by the entry in C9 (the number of C-H bonds in methane). The formula in Cell D14 is instructing Excel to sum or add up all the numbers in cells D8, D9, D10, D11 and 12.

Selected formula for the Excel spreadsheet are reproduced below in *Figure 805*. Similar Excel formulas should be entered in the other cells, namely: D9-D12, F8-F12.

Here are some suggestions for extending the spreadsheet:

- Use relative atomic masses from the IB Data Booklet to convert the enthalpy change of combustion into an enthalpy change (in kJ) per gram.
- Locate the density of methane and convert the enthalpy change into an enthalpy change (in kJ) per litre.
- Adapt the spreadsheet for any non-cyclic alkane, C_nH_{2n+2}, so the user simply enters n, representing the number of carbon atoms.

Bond energy.xls

	A	B	C	D	E	F	G	H
1	**Fuels - enthalpy changes of combustion**							
2								
3	Compound	CH4						
4								
5	Bond type	Bond energy	Number broken	Energy	Number formed	Energy released		
6		/kJ mol-1		/kJ mol-1		/kJ mol-1		
7	C-C	348	0	0	0	0		
8	C-H	412	4	1648	0	0		
9	C=O	743	0	0	2	-1486		
10	O=O	496	2	992	0	0		
11	O-H	463	0	0	4	-1852		
12								
13			Total energy	2640	Total energy	-3338		
14			(absorbed)		released			
15			kJ mol-1		kJ mol-1	-698		
16								
17								
18								
19								
20								
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Sheet1 Sheet2 Sheet3

Figure 805 Excel modelling of enthalpy changes of combustion

8.2 Data-logging

Data-logging is an electronic method of gathering and recording physical measurements; electrical sensors provide signals which are calibrated and recorded by a computer system.

Sensors and data loggers can be used in chemical experiments to measure and store the variations of physical quantities with time or with each other. Sensors and data loggers are very useful where the timescales of the experiments are either very long or very short, or when multiple data have to be acquired simultaneously. The use of an appropriate combination of sensors and data loggers to collect the required data and the use of real time graphing of the collected data allows you to spend more time on the analysis and evaluation of the data.

In the case of chemistry, data loggers and sensors could be used for experiments such as those involving measurement of temperature, pH, pressure or transmittance or absorbance of light through solutions.

The following are some examples of the use of sensors and data loggers in standard Chemistry experiments:

- the variation of pH during an acid-base titration
- the variation of temperature in a thermometric titration e.g. determining enthalpy of neutralization or enthalpy of precipitation
- the variation of light transmittance through thiosulfate solutions in the investigation of effects of concentration of acid on rate of reaction
- the variation of pressure during a chemical reaction where one of the products is a gas
- investigating the strength of intermolecular forces via evaporation
- monitoring enzyme activity via turbidity
- discharging electrochemical cells (simple batteries)
- verifying the gas laws and determining the gas constant

Data logging is particularly useful:

- for remote collection of data, on field work for example,
- for monitoring very fast changes, for monitoring very slow changes, for measuring changes very accurately,
- for measuring changes that are difficult to measure using conventional equipment such as high temperatures, infra red and ultraviolet radiation and gas volume,
- for measuring several variables at the same time.
- the data can be sent to a spreadsheet for display and analysis

All data loggers work with special software that enables gathered data to be stored, retrieved and displayed. Most of the graph plotting facilities have features that allow students to interact with the data and graphs, sometimes in a very powerful and sophisticated manner.

These features include:

- ability to change the parameters of the graph including axes, scales, limits and labels,
- measuring facilities to provide accurate data about specific points, the difference between points, areas under graphs, slopes of lines, and statistical data such as means, maximum and minimum readings,
- zoom facility to look closely at the fine detail of graphs,
- ability to superimpose several graphs on the same axes,
- the potential to draw secondary graphs derived from original data,
- opportunity to annotate graphs or data to draw attention to features of particular interest,
- ability to print tables or graphs, to save them and to export them to other electronic packages.

When designing a data logging activity you need to answer the following questions:

1. What variable do I want to measure?
2. What sampling rate and/or special start and stop options should I use?
3. How should the data be displayed?
4. How should the data be analysed?

Once the data have been collected and a graph drawn by the software, then a process of inquiry should begin. For example, some or all of the following questions may be appropriate:

- For each part of the graph, what was happening during the investigation?
- What caused that peak?
- What are the highest and lowest values?
- How large was a particular change and how long did it take?
- How quickly are the values changing?
- What is the underlying trend?
- What sort of pattern is present in the results?
- How does one variable seem to depend on another?

Your contribution, as the student, to the investigation must be evident such as in the selection of settings used by the data-logging and graphing equipment, or can be demonstrated in subsequent stages of investigation. It is important that if data-logging is used during an Individual Investigation that a print-out of the raw data is produced and included in your write-up.

8.3 Video cameras

Video cameras can also be used as data collection devices within chemical experiments. For example, this might be a suitable technique for investigating an oscillating reaction, such as the Briggs-Rauscher reaction or BZ reaction.

A video camera can be to record the timing of the colour changes. These data can then be compared to the voltage potential data and to our mathematical model to give a better understanding of what is happening in the reaction.

8.4 Phone applications

There are wide range of useful chemical applications for the iPhone. Here is a small sample:

Buffers <*https://itunes.apple.com/us/app/buffers/id306089755*> is a tool for designing buffer solutions for pH control. Buffers is useful both as a handy reference of available buffering agents and as an accurate, portable buffer calculator for chemical, biochemical and biological research. You may need a buffer if you are working with enzymes.

ChemiCal <*https://itunes.apple.com/us/app/graphbook/id348741481*> is a simple chemistry application that takes a given chemical formula and returns the mass of one mole of that chemical.

Chemical safety Data Sheets – ICS <*https://itunes.apple.com/us/app/chemical-safety-data-sheets/id405208132*>. This application displays International Chemical Safety Cards [ICSC] produced by the United Nations Environment Programme (UNEP), the International Labour Office (ILO), and the World Health Organization (WHO).

PhySyCalc <*https://itunes.apple.com/us/app/physycalc-for-iphone/id654457075*> an interesting scientific calculator (*Figure 806*) that lets you do full calculations but also lets you include the units. It also includes many useful mathematical functions, as well as a number of useful physical constants. Included also are the speed of light, and the mass of the electron, proton, and neutron, all with appropriate units, atomic weights, isotope weights, and isotope abundances.

Figure 806 PhySyCalc (App store on iTunes)

8.5 Simulations

There is a wide variety of software designed to simulate chemical experiments and industrial processes or to illustrate key chemical concepts. Some of these programmes are interactive, so that it is possible for the user to change the value of variables and observe consequent effects on the simulated system.

A particularly relevant type of simulation is the virtual experiment (*Figure 807*). In some cases you can start at the beginning with a choice of apparatus, and move on to decide on amounts of materials or operating conditions. The software tabulates data arising from the experiment and often generates an appropriate graph from it.

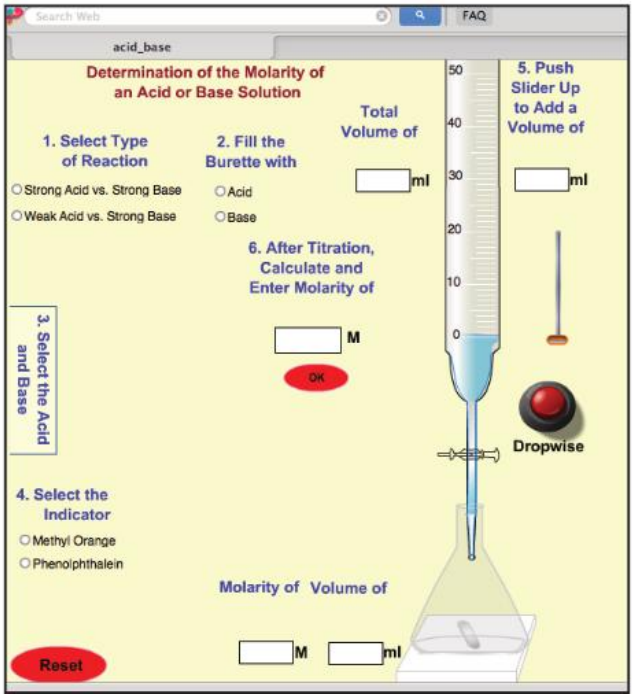


Figure 807 Titration simulation

from: <*http://group.chem.iastate.edu/Greenbowe/sections/projectfolder/flashfiles/stoichiometry/acid_base.html*>

This kind of software can be used by you to complement your practical work. It can be used as part of a pre-lab discussion to set the scene for the experiment, or to stimulate post-lab evaluation of experimental process and results.

8.6 Using Microsoft Word functions

8.6.1 Formatting tables

To insert a table using this method, simply click the Insert Table toolbar button when your cursor is positioned at the place in your document where you would like the table to begin. A grid will pop up allowing you to select how many rows and columns you would like your table to contain. Simply use your mouse to select the number of rows and columns by highlighting the boxes (text at the bottom of the grid will indicate what your selection is). When you have specified the correct number of rows and columns, simply click once, and your table will be inserted.

You can still customize your table after it is inserted by right-clicking on the table handle (the double-headed arrow at the top left corner of the table) and using the options on the shortcut menu to make changes.

Group	Ultra violet intensity/lux	5 days	10 days
Control	10	70.3 ± 2	90 ± 10.5
Test	10	60.4 ± 1.5	78 ± 7.9
Control	17	75.7 ± 8	100 ± 23
Test	17	52.2 ± 2	81 ± 26.7

Figure 808 Concentration of chemical X in sample after treatment

Look at the results in *Figure 808*. Two columns of data have been placed in the same cell, with the data arranged using the space bar.

Tables should be created with the correct number of rows and columns. You can also add new rows and columns to an existing table by right clicking on the table, selecting 'Insert' and choosing to insert new rows and columns above or below the existing rows or columns.

It is also possible to insert multiple rows/columns to a table by highlighting the number of rows/columns you require on existing rows/columns. For example, if you would like to add three columns to the left of your table, highlight the first three columns, right click and choose "Insert Columns to the Left".

8.6.2 Inserting symbols

When writing the report for your Individual Investigation you may need to use a number of special symbols from Microsoft Word. They can be accessed by selecting the Insert pull down menu and then choosing Symbol. Click on the symbol you want, then on 'Insert' and 'Close.' A small selection of mathematical and scientific symbols and their use is shown below in *Figure 809*.

Special symbol	Use or meaning
α	Proportionality
→	Reacts to form
Σ	Sum of
π	Pi (mathematical constant)
Ω	Omega (symbol of electrical resistance)
√	Square root
±	Plus or minus (indicates an absolute error or uncertainty)
°	Degree (used to indicate a temperature in Celsius)
÷	Division
⇌	Reversible reaction
≈	Approximately equal
λ	Wavelength
⊖	Standard conditions
θ	Angle

Figure 809 A selection of special symbols

8.6.3 Inserting charts and graphs

It is very easy to insert charts and graphs from Excel into Word. Select the Excel Spreadsheet so that it is highlighted and copy it by clicking "Ctrl+C." Mac users click "Cmd+C." In the Word document, click where you want the chart to appear. Paste the spreadsheet into the document by holding down the Ctrl key and hitting "V." On a Mac OS, click "Cmd+V."

With your cursor next to the data, click "Paste Options." To input the spreadsheet as a Word table, click "Keep Source Formatting." The chart will look like it did in Excel. Click "Match Destination Table Style" if you want the new graph to look like others you are using in the document.

8.6.4 Creating short cuts

You will probably have to write cm^3 a number or times for your reports. You type in cm^3 and then highlight the three and change into a superscript by selecting Format, Font and then Superscript. This is quite a long process and can be avoided by using a short cut:

Type cm^3 and format it to cm^3. Highlight it and choose Tools and AutoCorrect options. cm^3 will be present in the 'with box'. Type cm^3 in the 'Replace box' and select the 'Formatted text' circle. The cm^3 in the 'with' box will change to cm^3. Click 'Add' and 'OK'. Now when you type cm3 it will be automatically changed to cm^3. The short cut can be easily deleted.

8.6.5 The Equation Editor

If you want to include an equation in your report that includes division then you need to use the Equation Editor (*Figure 810*). Select the Insert pull down menu and then choose Object followed by Microsoft equation.

A special toolbar will also appear on your screen. Use the toolbar to select symbols, brackets, etc. to place in the box. You may also type numbers and letters into this box. At the top of the screen, a simplified toolbar lets you select font size (including subscript and sub-subscript), style, and alignment.

Figure 810 A screenshot of the Microsoft Equation Editor

Here is an example of a physical chemistry equation (Graham's law) written and then inserted using the Microsoft

Equation Editor: $\frac{rate\,1}{rate\,2} = \sqrt{\frac{molar\,mass\,1}{molar\,mass\,2}}$.

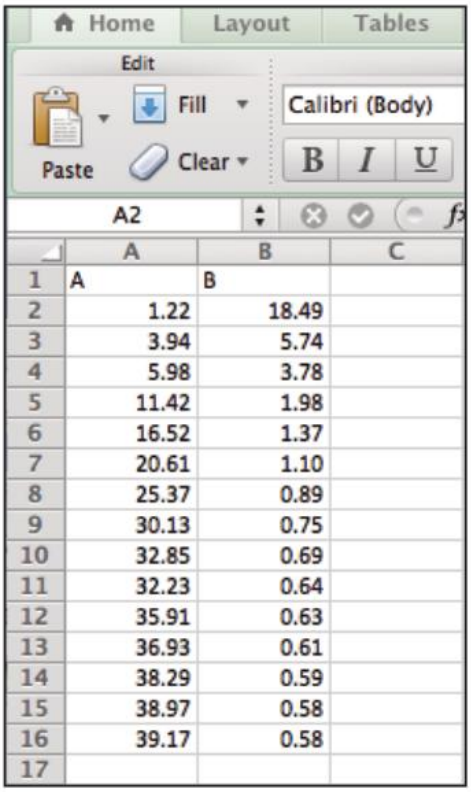
8.7 Using Excel functions

8.7.1 Plotting graphs

Graphing data on Excel

Type in your data, with your X axis data (independent variable) in the left-hand column, and your Y axis data (dependent variable) in the right column. Highlight your data (*Figure 811*). To the data is displayed to two decimal places Place your cursor over one of the data cells. Control click. In the drop-down menu that appears, choose "Format Cells." "Number" tab, and choose "Number" in the scroll-down menu. Type in "2".

With data still highlighted, choose the Chart Wizard icon in the menu bar (looks like a bar graph). Choose "Scatterplot" as your type of graph, and choose the version that has no line on it. Click At Step 2 (Source Data), click "Next." On Step 3 (Chart Options), give your graph a suitable title (your dependent variable versus your independent variable), and label your X and Y axes, making sure you include suitable units of measurement. Click "next," and on Step 4 (Chart Location), save graph as a "New Sheet." Change the name from "Chart 1" to a title that describes your graph (*Figure 812*). Click on "Finish."



	A	B
1	A	B
2	1.22	18.49
3	3.94	5.74
4	5.98	3.78
5	11.42	1.98
6	16.52	1.37
7	20.61	1.10
8	25.37	0.89
9	30.13	0.75
10	32.85	0.69
11	32.23	0.64
12	35.91	0.63
13	36.93	0.61
14	38.29	0.59
15	38.97	0.58
16	39.17	0.58
17		

Figure 811 Gas law data

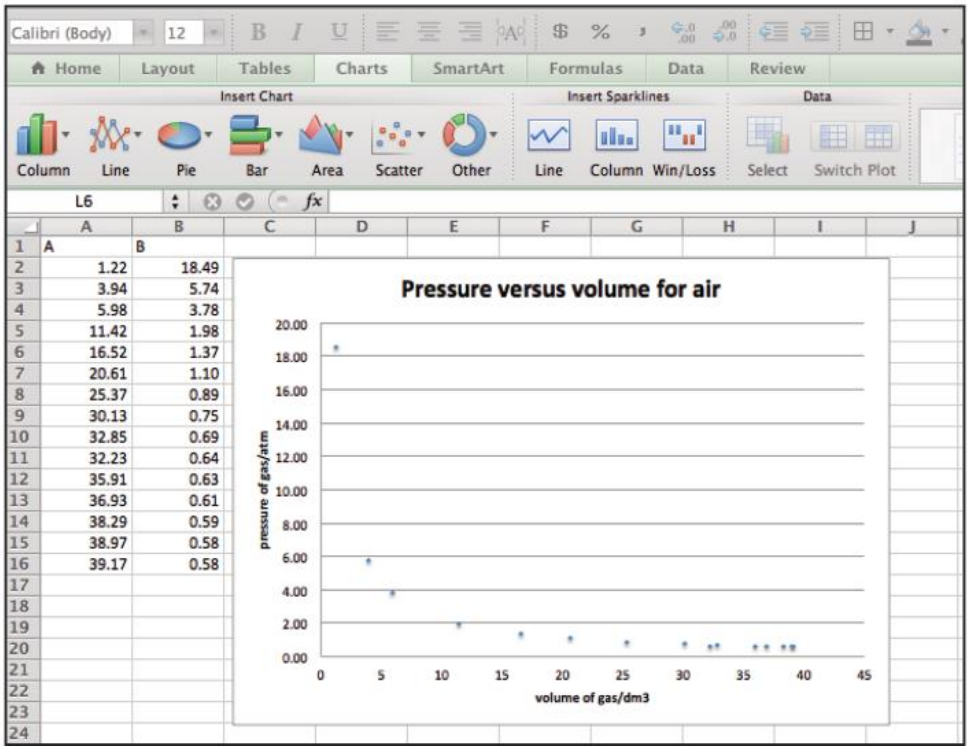


Figure 812 Gas law data plotted

8.7.2 Formatting graphs

To add a trend line and equation put your cursor directly over a data point, so that the point coordinates pop up. Control-click on this point and choose "Add Trendline" from the drop-down. For Trendline Type, choose the type of line that appears to best match the pattern your points make. This may be trial-and-error – you may have to do this more than once to find the best-fitting, but in this example a power trend line is appropriate. Click on the "Options" tab, and click on the "Display equation on chart" and "Display R-squared value on chart" at the bottom of the spreadsheet (*Figure 813*).

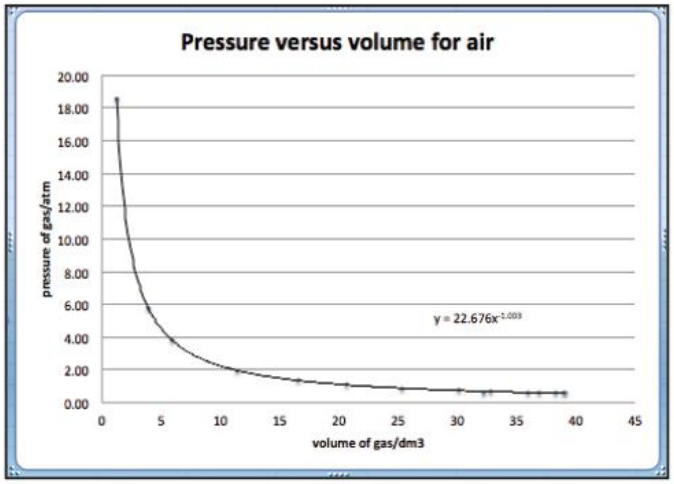


Figure 813 Gas law data plotted with power trendline

If you need to read X or Y values that are off the axes of your graph, you can forecast the trendline on your graph forwards or backwards to reach those values. Control-click on your trendline and choose "Format Trendline." Then, under "Options," you can forecast forwards or backwards however many units are needed. Then click "OK."

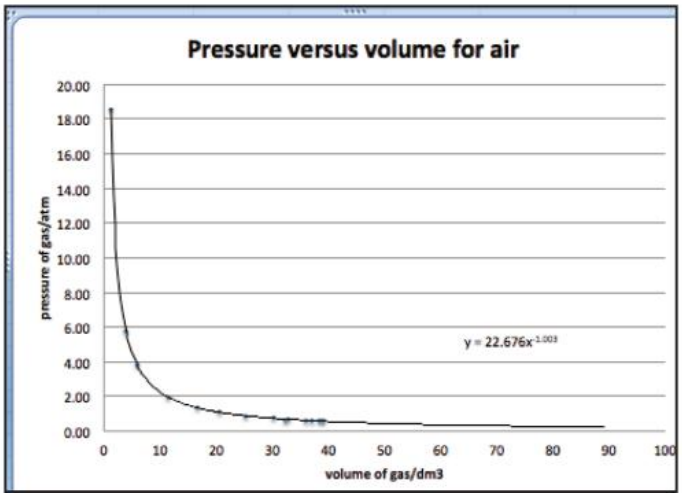


Figure 814 Gas law data with a forward forecast of 50 units

You can change the numbering system on your axes and add extra tick marks to your axes by formatting each axis. Put your cursor on the axis you want to format and Control-click, and choose "Format axis." See *Figure 814*.

You can choose to add additional tick marks to your scale by clicking on the "Colors and Lines" tab and clicking on the "Minor tick mark type" button of your choice. You can also choose the manner in which the tick marks are labeled. You can change the way the axes are labeled by choosing the "Scale" tab.

8.8 Using the Internet for research

8.8.1 Searching

The Internet is a vast store of scientific information that can be highly relevant, detailed and up to date. It can provide information ranging from data on atmospheric carbon dioxide levels and stem cell medical research to photographs from the Hubble space telescope.

Unfortunately, much information can also be irrelevant, and you can waste much time on unproductive searches. Search engines such as Yahoo, Google, Altavista and Ask Jeeves produce best results when the search request is made as specific as possible, using their advanced search facilities.

Many search engines, such as Google, use a + sign to link words in a single site together, or contain advanced search buttons to match the site with all the words that are being searched for.

For example, typing in nanotechnology research + singapore will only report web sites that contain information about nanotechnology research in Singapore.

8.8.2 Applets

The Internet is also a rich source of animated images, called applets or small applications, which are programmes designed to run in a web page. These include the following.

Simulations of experiments

These are often ones which are difficult to carry out in the laboratory, such the effect of temperature on a chemical equilibrium (*Figure 815*). Experiments might also be chosen that take a long time to set up or require expensive equipment. The applet simulation can generate results very quickly, and so allow you to spend most of your time thinking about the data rather than recording it.

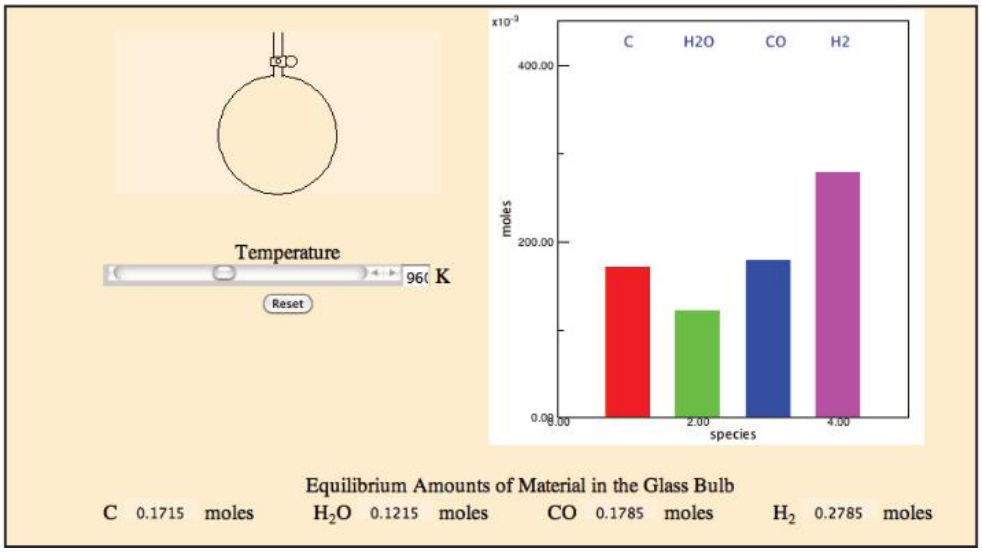


Figure 815 Chemical equilibrium simulation

from <*http://www.chm.davidson.edu/vce/Equilibria/Temperature.html*>

Visualisation of ideas, concepts and mechanisms

Animated and three dimensional images can often provide easier access to concepts such as organic reaction mechanisms, which may be very hard to grasp when described by text and a series of two dimensional diagrams in a book. Concepts such as simple collision theory the can also be illustrated very easily.

The main technologies for creating applets are Java and Shockwave. Java file or files that make up an applet are called .class files, and they will automatically run in most modern web browsers. Shockwave technology produces applets or animations specifically for browsers: these are called .swf files. More modern web browsers will automatically support Shockwave, but others will need a readily available 'plugin' or small helper programme available from www.shockwave.com. Search engines can be used to find applets, by using their advanced facility to look, for example, for kinetic simulation and applet.

8.8.3 Retrieving scientific papers

During your Individual Investigation you might want to find out about previously published chemical or biochemical research. This can be done by performing a search on a public database known as PubMed (see *Figure 816*). PubMed is a bibliographic database maintained by the National Center for Biotechnology Information in the United States. It is also known as Medline or Entrez. It contains references on abstracts on life sciences and biomedical topics, but some of these may be relevant to a Chemistry Individual Investigation.

To search PubMed use your browser to navigate to *<http://www.ncbi.nlm.nih.gov/entrez>* on the Internet.

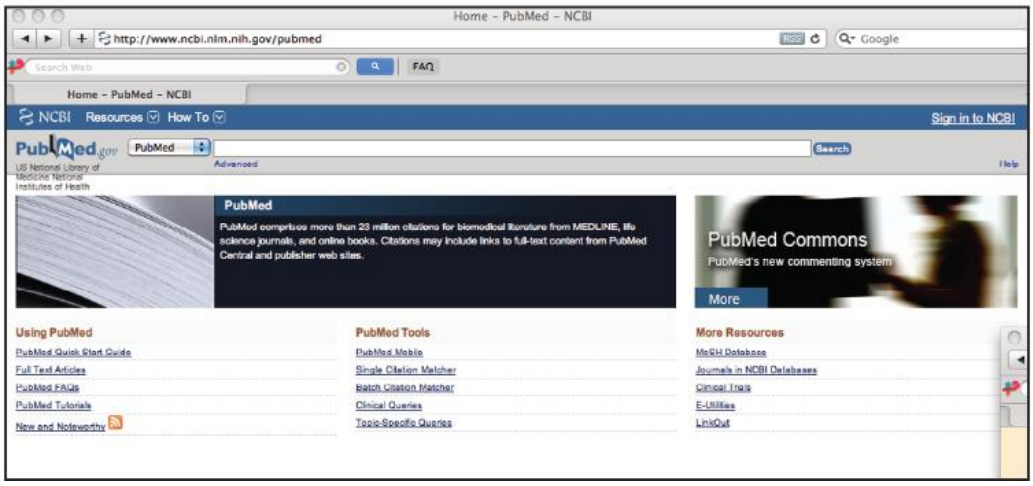


Figure 816 The initial PubMed search window

Then type in a name, for example Briggs Rauscher which is the name of an oscillating reaction. Very rapidly a Results list is generated on the screen (see *Figure 817*).

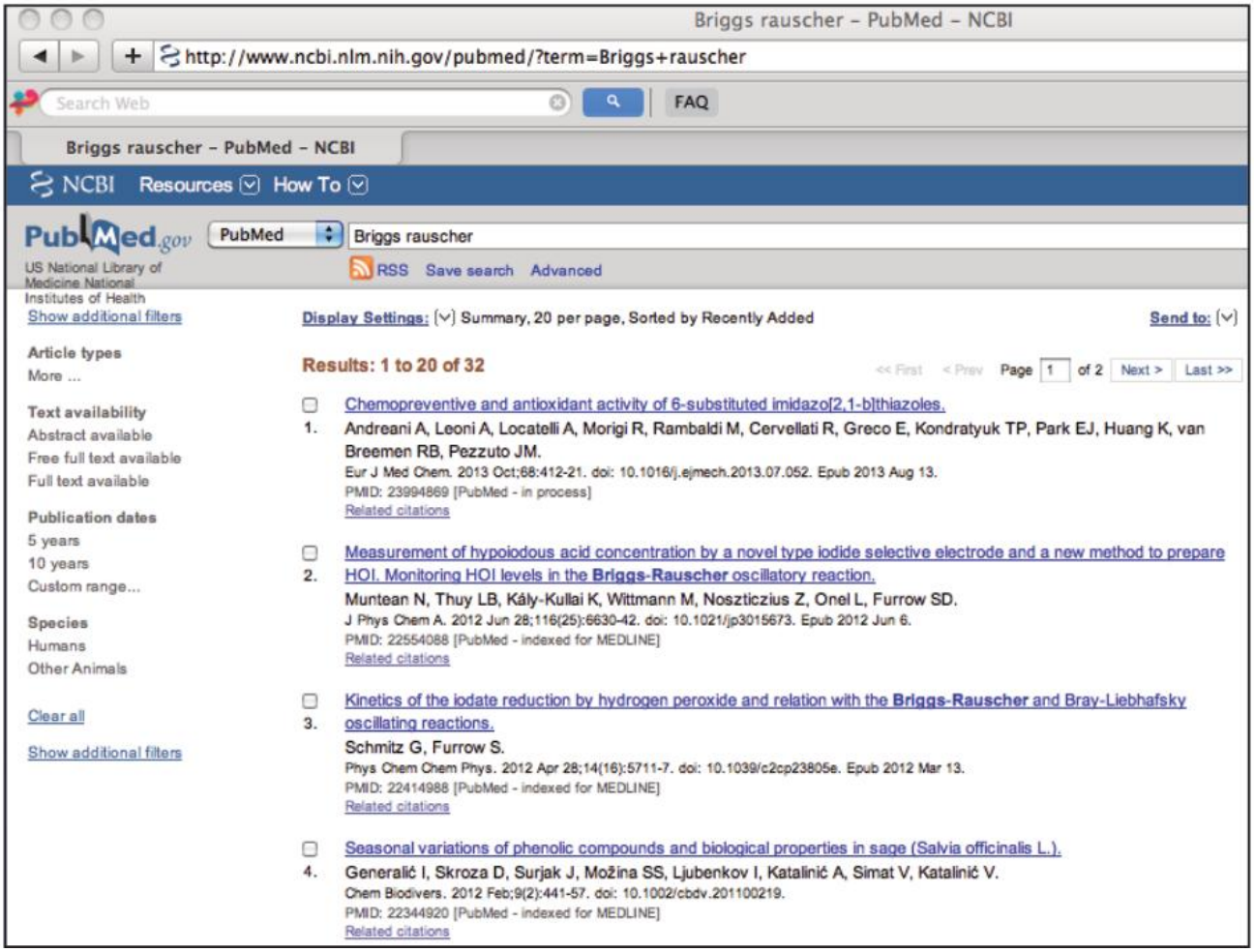


Figure 817 The initial result of a standard Pub Med search for Briggs Rauscher reaction

To move through the Results pages, simply click Next located in the top right of the screen. The authors' names are clickable hyper links. Clicking on them will display a summary of the selected research paper

You can save the files on to your computer's hard drive by choosing your browser's File → Save As option. Queries to PubMed can be narrowed down by predefining different attributes in different fields before running your search. If you want to limit your PubMed search to recent review articles about the Briggs Rauscher reaction then follow these steps:

- Type in Briggs Rauscher in the For window of PubMed.
- Do not press the 'Go' button, but click on Limits located just below the arrows of the pull-down menu of the search window.
- The limits search window appears.

Absolute error

An absolute error is an error expressed in physical units.

Accuracy

A measure of the total error in your measured value. The accuracy of a measurement depends on the experimental techniques and equipment used. Accuracy can be improved by removing or minimising error.

Anomalous data

Data with unexpected values that do not match the relationship predicted by the hypothesis. Anomalous results can be due to experimental error.

Calibration

Standardisation of the measurement scale of an instrument or apparatus.

Conclusion

A conclusion is an interpretation of experimental data. The conclusion should, if possible, show whether the data support or reject any hypothesis put forward.

Controlled variable

Controlled variables are potential variables which are fixed and not allowed to vary during an investigation.

Dependent variable

These are the variables that are measured during an investigation.

Error

An error in a measurement is the difference between the measured value and the true value.

Evaluation

This involves the consideration of all errors, random and systematic, which may affect the results, identifying weakness and limitations in the method, calculating the total error present in the results and explaining how the errors can be minimised.

Extrapolation

To estimate (a value of a variable outside a known range) from values within a known range by assuming that the estimated value follows logically from the known values.

Fair test

A test in which one variable is manipulated or changed.

Hypothesis

A tentative or interim explanation for an observation, phenomenon, or chemical problem whose predictions may be tested by further investigation.

Independent variable

An independent variable is a one whose values are chosen by the experimenter.

Inference

An inference is a tentative conclusion drawn from a series of observations. It may lead to the formulation of a hypothesis.

Interpolation

To estimate a value for a variable of between two or more known values. This is frequently done graphically.

Law

A scientific law is a generalisation that scientists make from an extensive body of research findings. A useful scientific law can be used to accurately predict what will happen in a range of situations.

Limitations

The restrictions of a particular experimental technique or set of apparatus. Limitations encountered during an investigation could influence the results and would need to be addressed in the evaluation.

Literature value

A value from the chemical literature of a physical constant or experimental measurement.

Observation

Observations are what changes can be measured, seen, heard, smelt, tasted or felt during an investigation.

Precision

The precision is the total amount of uncertainty present in a measurement.

Percentage error

A percentage error is an error expressed as a percentage of the value measured or of the true value.

Prediction

Predictions are a consequence of a hypothesis and descriptions of the results you expect to obtain from an investigation.

Processed data

Raw data which have been organised and/or mathematically or graphically transformed.

Propagation of errors

Calculating the overall error from a series of mathematical operations.

Qualitative data

Qualitative data refers to observations made without measurements.

Quantitative data

Quantitative data refers to numerical measurements.

Replication

This involves repeating a test, or observation, a number of times.

Random error

Random errors are present every time a measurement is recorded. Their effects can be reduced by repeating the measurement and averaging.

Raw data

This is data which have not yet been processed or analysed.

Reliability

A measure of the confidence that can be placed in a set of observations or measurements. The reliability of a set of observations or measurements depends on the number and accuracy of the individual observations or measurements. Reliability can be improved by replicating observations and measurements.

Resolution

The size of the smallest increment which can be shown on the measurement display. On a digital display, it is the value of the least significant digit.

Risk assessment

A consideration of the possible safety hazards that could be encountered during an investigation.

Sensitivity

The ratio between the change in measurement to the change in measured quantity.

Significant figures

The significant figures in a number are those that are meaningful.

Standard deviation

A measure of dispersion, providing an estimate of the average deviation of data points from the mean.

Systematic error

An error which biases your measurements in some predictable but perhaps unknown or unrecognised way. Systematic errors cannot be reduced by repeating the measurement and averaging.

Tests

Investigations are usually composed of a number of tests where one variable is manipulated or changed.

Theory

A set of statements or principles devised to explain a group of facts or phenomena, especially one that has been repeatedly tested or is widely accepted and can be used to make predictions.

Trend

The general direction, tendency or patterns shown by a set of measurements or observations.

Trueness

Refers to the closeness of agreement between the average value obtained from a large series of test results and an accepted true.

t-test

A statistical test used to compare the means of two independent samples from a normally distributed population.

Uncertainty

An uncertainty is the range that will likely contain the true value of whatever is being measured.

Validity

A measure of the confidence that can be placed in a conclusion. The validity depends on factors such as the range and reliability of observations and measurements. Statistical tests may be used to place a value on the reliability of data.

Variable

The conditions or factor that can vary and may be varied during an experiment. As far as possible only one variable should be changed or manipulated at a time.

Variability

The degree to which the observations or measurements differ from one another.