ROYAL SOCIETY OF CHEMISTRY

Analytical chemistry in Ireland

A teaching and learning resource

Science Foundation Ireland sfi For what's next

SMART FUTURES

This work was produced as part of a community project, with contributions from the Royal Society of Chemistry (RSC) members and staff, industry partners, Science Foundation Ireland and, most importantly, members of the teaching community in Ireland.

We would like to acknowledge the following books and teaching materials that were used as reference guides:
(1) *Leaving Certificate Chemistry Syllabus (Ordinary Level and Higher Level)*, National Council for Curriculum and Assessment (NCCA), **curriculumonline.ie/Senior-cycle/Senior-Cycle-Subjects/Chemistry**
(2) D Kennedy, *Chemistry Live!*, Folens Educational Publishers, Dublin, 2014
(3) *Teacher's Reference Handbook Chemistry,* Module 1, Atomic structure and trends in the periodic table of the elements pg. 4, 24–25, 39 and Module 10 Some Irish contributions to chemistry pg. 1–26, Department of Education and Science, Ireland, 2000, **education.ie/en/Schools-Colleges/Information/Curriculum-and-Syllabus/Senior-Cycle-/Syllabuses-and-Guidelines/lc_chemistry_teachers_guide.pdf**
(4) J McCarthy and T White, *Understanding Chemistry Leaving Certificate,* 2nd edition, Education Company of Ireland, Ireland, 2004

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Welcome

A supporting guide

Ireland is continuing to invest in its rapidly expanding pharmaceutical and related manufacturing sector. This includes biological and chemical based industry and third-level research initiatives across the country. As this area of the economy develops even further, new researchers and talented individuals with the right skills and knowledge are required.[1]

Essential to any research and development is a core understanding of analytical chemistry. We developed this resource to support secondary school teachers to develop the skills.

We provide curriculum-linked activities, inspiring real-life career stories and application-based assessment to develop the necessary scientific inquiry skills through four suggested student projects.

For more information on chemistry and related science, technology, engineering and maths (STEM) careers and further study, go to the 'A future in chemistry' website **edu.rsc.org/future-in-chemistry** for chemistry job profiles. You can find a dedicated brochure for post-16 options in Ireland here **edu.rsc.org/future-in-chemistry/not-a-student/teachers-and-careers-advisers/explaining-the-benefits-of-a-chemistry-career**

Other useful resources are available through Science Foundation Ireland's (SFI's) Smart Futures programme **smartfutures.ie**

References

1 Landscape of the European Chemical Industry 2020 report, Cefic **cefic.org/a-pillar-of-the-european-economy** (accessed 22 June 2020)

Information kindly supplied by Biopharmachem Ireland who are a business association within Ibec representing the biopharma and chemical sectors. More information available at **biopharmachemireland.ie**

Contents

How to use this resource

In this resource you will find a variety of content including worksheets, project based learning tasks and contextualisation stories. We have segmented all the material so that it can be used in a mix-and-match style that works best with your particular teaching approach, student cohort and learning objectives. To support you in easily sourcing the content you need, we have divided it into colour-coded subsections.

There are distinct subsections designed to help plan and run a series of lessons and set your class a group project designed to build student skills and contextual awareness in an area relating to analytical chemistry.

The **Introducing scientific skills** sections contain suggested teacher lesson ideas and student information sheets to provide the theoretical background to key analytical topics. In the **Quantitative chemistry ideas** section, you will find further teaching ideas and students examples to cement learning.

The **Applying scientific skills** sections contain guidance for the student projects. Each project embeds a student skill and a suggested portfolio assessment. To expand on that learning, students can read stories about the work of Royal Society of Chemistry member's in the **Careers and industry stories** section.

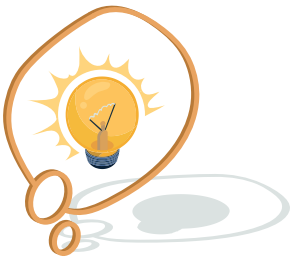
Introducing scientific skills

Introduction to spectroscopy

Concise information sections for students that can be used at the beginning of a topic to explain the different spectroscopic techniques.

Themed lesson guide

Background information and planning support for teachers who would like to run the two–three lesson series which lays the groundwork for each of the student projects. Includes a step by step preview of the associated PowerPoint presentations.



Quantitative chemistry ideas

An assorted compilation of student support sheets and strategies for teaching the quantitative aspects of analytical chemistry. These have been kindly donated from within our education community.

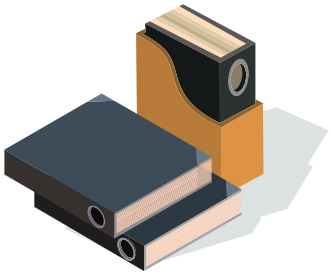
Applying scientific skills

Teacher's project guide

A complementary teacher's guide for each **student project** including supporting references and answers.

Class project instructions

Step by step guides for each student project to help organise the class group. Also includes relevant links to **careers and industry stories** to help contextualise each topic within Ireland's analytical chemistry sector.



Student project portfolio

The project portfolio helps to structure and document the learning and is ideal for transition year students. A student project portfolio for each project is available for download from the Royal Society of Chemistry website **rsc.li/3p00LfI**

Careers and industry stories

Stand-alone contextualisation support for teaching analytical chemistry from Royal Society of Chemistry members. Real-life stories about how analytical chemistry helps Ireland's scientists tackle problems in industry today. Each story comes with discussion questions.

Applied scientific skills with four student projects

1. Observation and inference – **Emission competition** p17
2. Accuracy and precision – **Phone-y science** p37
3. Evaluating a scientific model – **Building a mass spectrometer** p59
4. Research and analysis – **The sunshine factor** p81

This entire resource can be downloaded in PDF from **rsc.li/3p00LfI** so that all sections are accessible to you on a whiteboard. Teacher and student content is clearly marked so you can use each section as needed.

Introduction to spectroscopy

What's in this section?

Student summaries and links to supporting documents which help teachers bring instrumentation into the classroom.

Who is it for?

This section is directed at students but will also assist teachers by providing an overview of the instrumentation and their links to the syllabus.

What is analytical chemistry and what use is it?

The Leaving Certificate Chemistry syllabus requires students to be able to describe and explain some different analytical methods, as well as apply this knowledge to identify and quantify materials.

Analysing something means to examine it closely, to understand it at a basic structural level.

Analytical chemistry can be described as the science of finding out what a material is made of and how much of it there is. Using high-tech pieces of equipment (instrumentation) makes this job simpler for scientists and much more accurate, and all modern laboratories use them.

A key distinction to be aware of in analysis is what is being measured; it is either the quantity or quality of something. Quantitative analysis measures the amount of something (eg a microgram of a drug) while qualitative analysis is related to a scientific descriptor (eg highly flexible).

Analytical chemistry is fundamentally important to all branches of chemistry, extending its influence to the biological sciences and geology.

Analytical chemists use their knowledge of chemistry, instruments, computers and statistics to solve problems. The tools they use help them 'see' in the invisible molecular world. Analytical chemistry is important for exploring new materials, finding more accurate or more sensitive ways to analyse existing materials and for pushing the boundaries of what we can know.

In Ireland, analytical chemistry is the backbone of the pharmaceutical and life sciences. Ireland is home to nine of the top 10 pharmaceutical companies in the world. It is also the 8th largest producer and the 5th largest exporter of pharmaceuticals globally.

A total of 120 pharmaceutical companies are based in Ireland, with products that make up half the total goods exported from the country. These sectors are currently contributing €3 billion in capital expenditure to the economy.[1]

There are a variety of challenging and interesting careers available in these industries to those with a strong background in analytical chemistry.

The study of analytical chemistry in the classroom can seem limited by not having the newest equipment or instrumentation, however, through simple experiments and scientific enquiry you can explore the theory and application of the fundamental analytical chemistry concepts which will be critical for actually using these pieces of high-tech equipment during a career in the industry.

What skills will you need in 2026? See chemistryworld.com/careers/what-skills-will-you-need-in-2026/1017241.article

References

1 All information on Ireland pharmaceutical and life sciences industry obtained from IDA Ireland, **idaireland.com**

The role of instrumentation

Analyst using UV-visible spectroscopy.

Instruments or instrumentation (a collective term for instruments) were developed to enhance scientific investigations.[1] For example, identifying a white powder found at a crime scene.

Often the physical properties of a substance are used to give us further information about the substance's chemical properties or even the structures of the chemicals it contains.

The chemical properties of substances are defined by their reactions, so by reacting them with other substances or stimuli like heat you can measure their chemical characteristics.

Spectroscopy is an example of this. It seeks to study how electromagnetic radiation interacts with matter, or more specifically how matter and light interact to identify, detect and quantify the chemical properties of a substance.

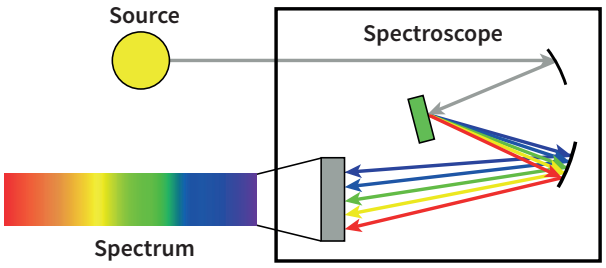
The spectroscope, and wider field of spectroscopy, have evolved considerably since early opticians, astronomers and philosophers first mused on the nature and composition of light and matter.

There is a rich history behind this technique, you can find a detailed timeline of discoveries and inventions by a variety of key scientific figures on the Spectroscopy Online journal's website **spectroscopyonline.com/timeline-atomic-spectroscopy**

A spectrometer is any instrument used to probe a property of light, typically its wavelength, frequency or energy in a particular region of the electromagnetic spectrum. The property being measured is usually intensity of light, but other variables like polarisation can also be measured.

A spectroscope is a device that measures the spectrum of a source of light. Early versions had a slit, a prism and a screen with markings to indicate various wavelengths or frequencies; later these were calibrated to electronic detectors. The apparatus Isaac Newton used in his work on the spectrum of light in 1666 can be considered a crude spectroscope, but Gustav Kirchhoff and Robert Bunsen were the first to discover elements using spectral analysis in 1860–1861.

A spectrograph is an instrument that separates incoming light by its wavelength or frequency and records the resulting spectrum in some kind of multichannel detector, like a photographic plate. Many astronomical observations use telescopes which serve as spectrographs.[2]



Spectroscope and spectrograph

References

1 Typically, instruments are used to measure a physical property of a substance, ie a property that can be measured without changing the substance's composition

2 D W Ball, *Field Guide to Spectroscopy*, SPIE Press, Bellingham, 2006

What is spectroscopy?

Spectroscopy is the study of the way light (electromagnetic radiation) and matter interact. There are a number of different spectroscopic techniques, but the basic principle shared by all is to shine a beam of a particular electromagnetic radiation onto a sample and observe how it responds to such a stimulus. This allows scientists to obtain information about the structure and properties of matter.

Excitation

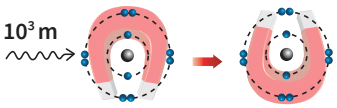
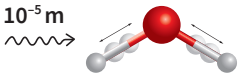
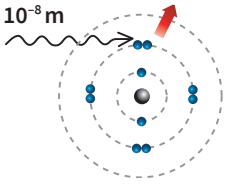
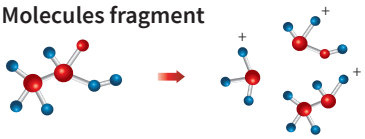
When matter absorbs electromagnetic radiation, the change that occurs depends on the type of radiation, and therefore the amount of energy, being absorbed. Absorption of energy causes an electron or molecule to go from an initial energy state (ground state) to a high-energy state (excited state), which could take the form of increased rotation, vibration or electronic excitation. By studying this change in energy state scientists are able to learn more about the physical and chemical properties of the molecules.

The energy states are said to be quantised because a photon of precise energy and frequency (or wavelength) must be absorbed to excite an electron or molecule from the ground state to a particular excited state.

Because molecules have a unique set of energy states that depend on their structure, infrared (IR), ultraviolet (UV)-visible and other types of spectroscopy will provide valuable information about the structure of the molecule:

- radio waves can cause nuclei in some atoms to change magnetic orientation and this forms the basis of a technique called nuclear magnetic resonance (NMR) spectroscopy;
- molecular rotations are excited by microwaves;
- electrons are promoted to higher orbitals by UV or visible light;
- vibrations of bonds are excited by IR radiation.

Comparison of common spectroscopy techniques and the wavelength of radiation used in each. Note: mass spectrometry doesn't use electromagnetic radiation and is a non-spectroscopic technique

TECHNIQUE	RADIATION		WHAT CAN IT SEE?
NMR spectroscopy	Radio waves (10^3 m)	Nuclei flipping magnetic spin 	How neighbouring atoms in a molecule are connected together, as well as how many atoms of these types are present in different locations in the molecule.
IR spectroscopy	IR (10^{-5} m)	 Note: Molecule vibrations	The functional groups that are present in a molecule.
UV visible spectroscopy	UV (10^{-8} m)	 Note: Electrons promoted to higher state energy	Double bond systems such as carbonyl groups (alternating single and double bonds) in organic molecules.
X-ray crystallography	X-rays (10^{-10} m)		How all the atoms in a molecule are connected in a three-dimensional arrangement.
Mass spectrometry	Non-spectroscopic technique	Molecules fragment 	The mass to charge ratio of the molecular ion (ie the molecular weight) and the fragmentation pattern, which may be related to the structure of the molecular ion.

Ultraviolet (UV)–visible spectroscopy

Syllabus links

- UV absorption spectrometry as a quantitative technique involving the absorption of UV light.
- Quantitative determination of organic compounds (eg drug metabolites and plant pigments).
- A brief description of the principles of UV spectroscopy.
- Environmental chemistry: colorimetry in water analysis.

How does it work?

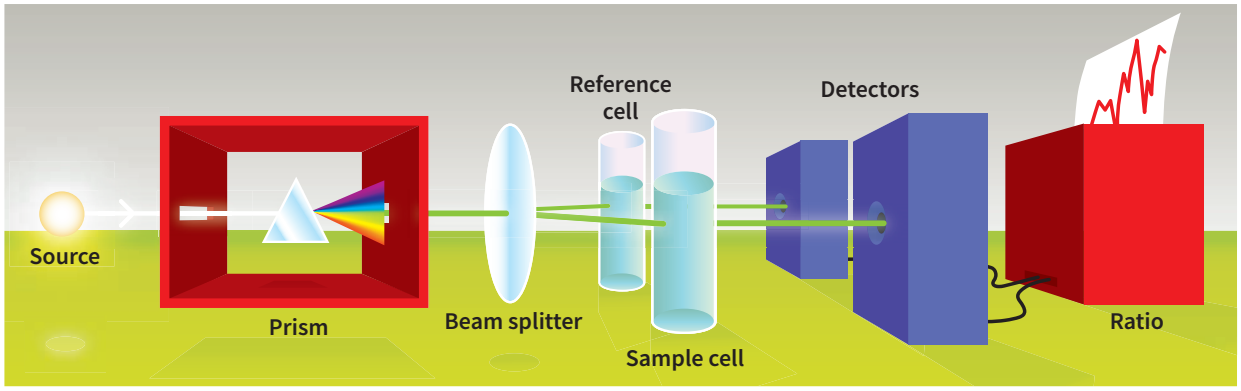
Absorption of visible and UV radiation is associated with excitation of electrons, in both atoms and molecules, from lower to higher energy levels.

Because the energy levels of matter are quantised, only light with the precise amount of energy to cause transitions from one level to another will be absorbed.

It is possible to predict which wavelengths are likely to be absorbed by a coloured substance. When white light passes through or is reflected by a coloured substance, a portion of the mixed wavelengths is absorbed.

The remaining light will then assume the complementary colour to the wavelength(s) absorbed. This relationship is demonstrated by the colour wheel shown below. Complementary colours are diametrically opposite each other.

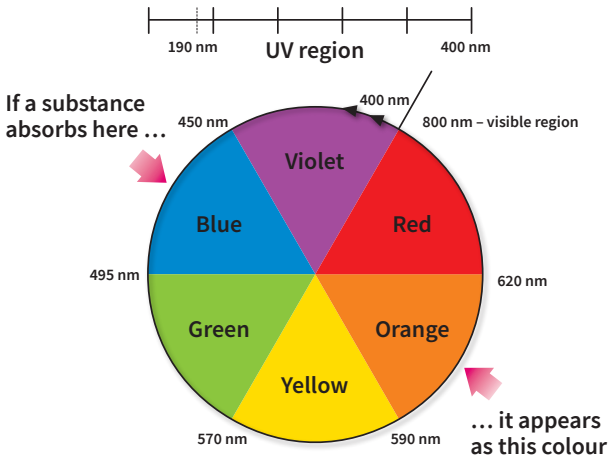
Schematic diagram of a UV-vis spectrometer



UV–visible spectrometers can be used to measure the absorbance of UV or visible light by a sample, either at a single wavelength or by performing a scan over a range in the spectrum. The UV region ranges from 190 to 400 nm and the visible region from 400 to 800 nm.

A colorimeter is an instrument that measures the absorbance of light by a sample at a fixed wavelength only, usually with a single LED light source.

Colorimeters and spectrophotometers both measure sample absorbance to determine a sample's concentration when compared against a **known standard**[1]; the technique can be used both quantitatively and qualitatively for analysis.



Colour wheel of UV light

References

1 A known standard is a material that contains an accurately known concentration of a substance. See the interactive lab primer – standard solution **edu.rsc.org/resources/standard-solution/2257.article**

Infrared (IR) spectroscopy

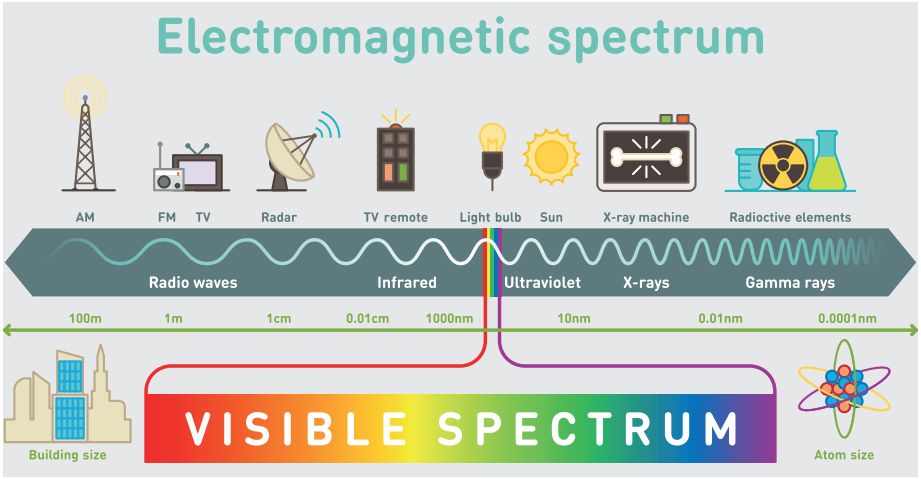
Syllabus links

- IR absorption spectrometry as a 'fingerprinting' technique involving absorption of IR radiation (reference to molecular vibrations not required).
- Identification of organic compounds (eg plastics and drugs).
- A brief description of the principles of IR spectroscopy.

How does it work?

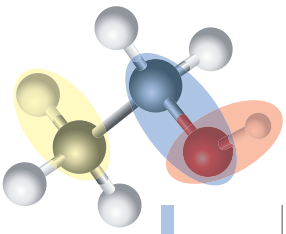
IR is a type of spectroscopy that involves the absorption of IR waves by molecules. Exciting the molecules causes them to bend, stretch and contort in different ways, depending on their structure.

The resultant pattern can be measured by IR spectroscopy, giving us information about the structure. We can also match up the absorption spectrum of an unknown compound with a known compound in order to identify it.

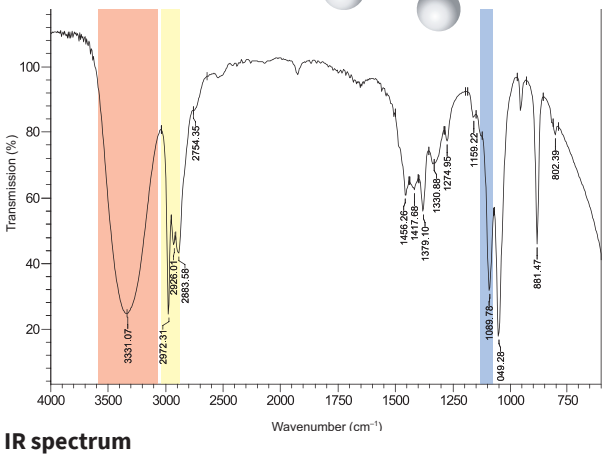


The range of wavelengths and frequencies of light – the electromagnetic spectrum. Shown left with relative size comparison

Ethanol molecule



An IR spectrum is essentially a graph plotted with the IR light absorbed on the y-axis against wavenumber (cm^{-1}) on the x-axis.
IR waves have a longer wavelength than the waves in the visible and UV region, as shown in the diagram on the right.

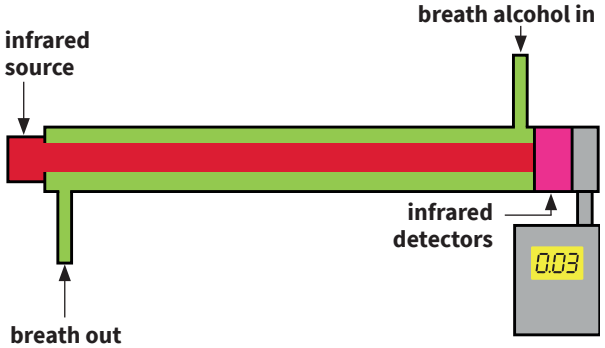


IR spectrum

The uses and applications of IR spectroscopy

IR spectroscopy is used by police forces across the world in alcohol breathalysers. The C–O bond in alcohol absorbs at around 1060 cm^{-1} and this is what the breathalyser detects.

It is also used to identify functional groups within molecules associated with drugs. This can be used when checking an athlete's blood for banned substances, for example.



Schematic of how a breathalyser uses IR to detect alcohol bonds in breath

Nuclear magnetic resonance (NMR) spectroscopy

NMR spectroscopy is used to determine the molecular structure of unknown compounds. The technique provides chemists with information on the electronic environment in which the nuclei of atoms are present in the molecule, and they use this information to determine the molecule's chemical structure. The most recognisable application of this technique would be its medical use in the form of magnetic resonance imaging (MRI).

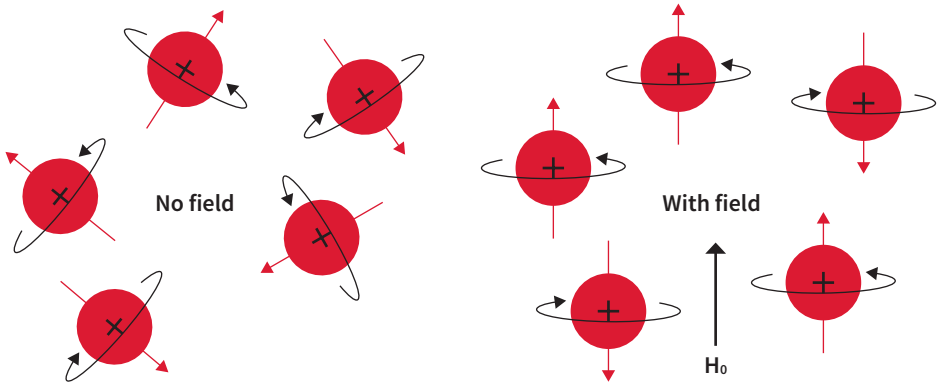
NMR spectroscopy does not currently feature in the Leaving Certificate syllabus, but it is a key analytical technique that can be used alongside other spectroscopic methods to identify compounds.

How does it work?

The principle behind NMR is that nuclei with an odd mass or odd atomic number have nuclear spin (in a similar fashion to the spin of electrons). This includes hydrogen (^{1}H) and carbon-13 (^{13}C) (but not ^{12}C) which means that they have the potential to act like tiny bar magnets when exposed to a sufficiently large magnetic field (the NMR spectrometer) and an energy transfer is possible between the base energy of the nucleus to a higher energy level.

Just as electrons with opposite spin pair up with each other in bonding orbitals, a similar thing happens with protons and neutrons in the nucleus. The nuclear magnet can have two alignments, of low energy and high energy. To make the nucleus change to the higher energy alignment, energy must be supplied. For NMR, the energy absorbed corresponds to radio frequencies.

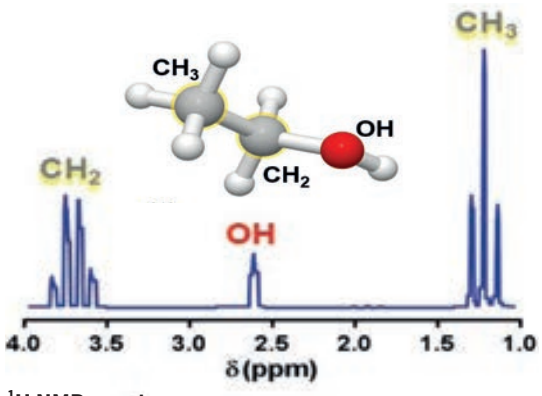
The precise frequency of energy absorbed by the nucleus depends on the environment of the nucleus, which is dependent on the other nuclei and electrons in its neighbourhood. So, by placing the sample being examined in a strong magnetic field and measuring the frequencies of radiation it absorbs, information can be obtained about the chemical environments of nuclei in the molecule. NMR spectroscopy is particularly useful for identifying the positions of hydrogen atoms in molecules, which provides us with information about a molecule's structure.



Nuclei flipping magnetic spin in the presence of the magnetic field applied in NMR spectroscopy

NMR spectra

The NMR spectrum can be measured for many nuclei but the most common are ^{1}H and ^{13}C.



^{1}H NMR spectrum

^{1}H peaks corresponding to each unique hydrogen environment in the proton NMR spectrum of ethanol

Supporting videos
edu.rsc.org/resources/chemistry-vignettes-nmr-theory/1340.article
edu.rsc.org/resources/nuclear-magnetic-resonance-nmr-spectroscopy/11330.article

Mass spectrometry (MS)

Syllabus links

- Using a mass spectrometer to determine the relative atomic mass of atoms.
- Calculating relative atomic mass from abundances of isotopes.
- Instrumentation in organic chemistry.
- Fundamental processes in mass spectrometry.
- Analysis of gas, waste water and drugs.

How does it work?

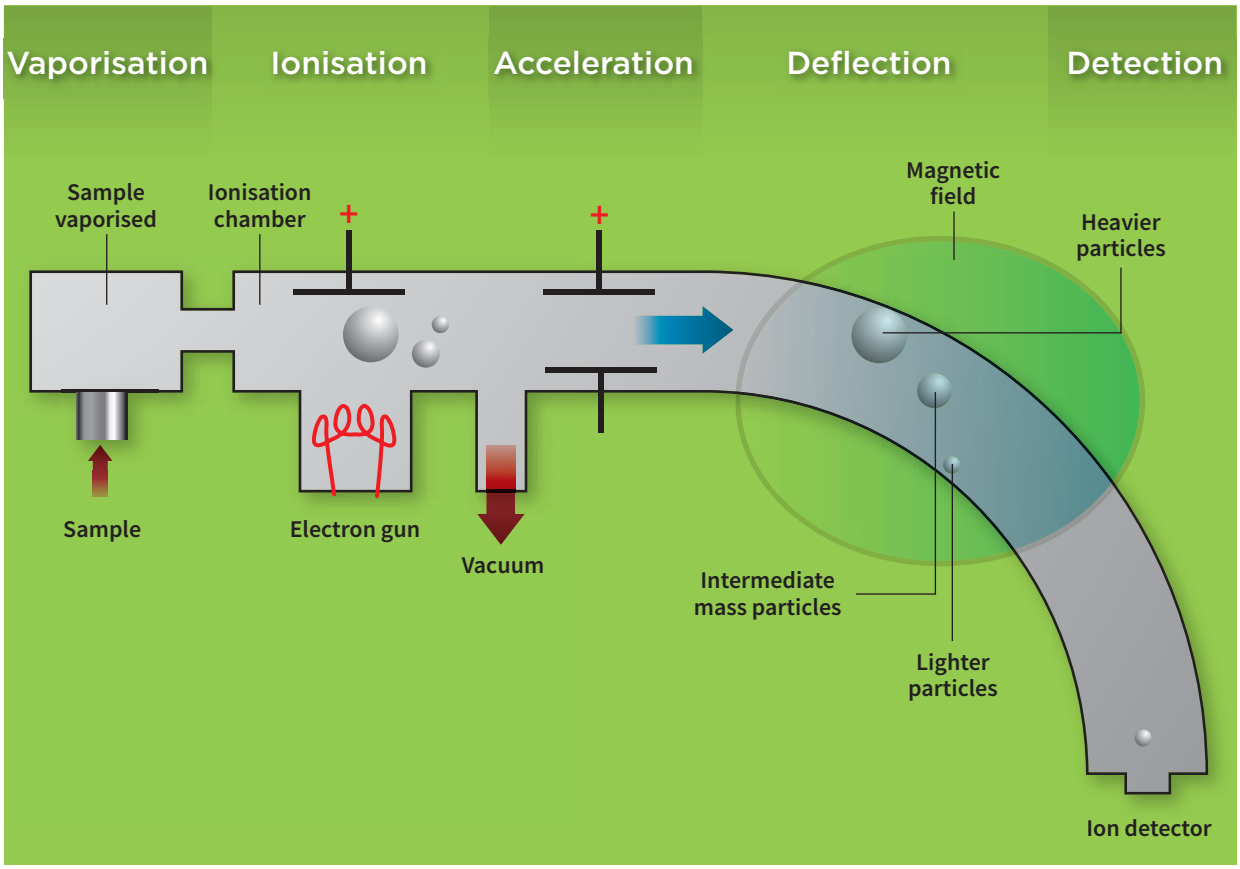
MS is a very powerful analytical tool that can provide information on both molecular mass and molecular structure. This technique is about 1000 times more sensitive than other analytical techniques such as IR or NMR spectroscopy.

Essentially, a mass spectrometer performs three functions:

1 Creates positive ions from a neutral sample.

2 Separates the ions according to their mass/charge (m/z) ratio.

3 Measures the relative abundance of ions and their relative masses, this information is translated into a mass spectrum.



Schematic of mass spectrometer highlighting the main processes

In a mass spectrometer, the sample is vapourised so that a stream of positively charged ions travels along an applied magnetic field. Next, the sample must be ionised by bombarding the sample with high-energy electrons from an electron gun.

These knock off an electron to produce a positive ion. Consider a helium atom:

$$He(g) + e^- = He^+(g) + 2e^-$$

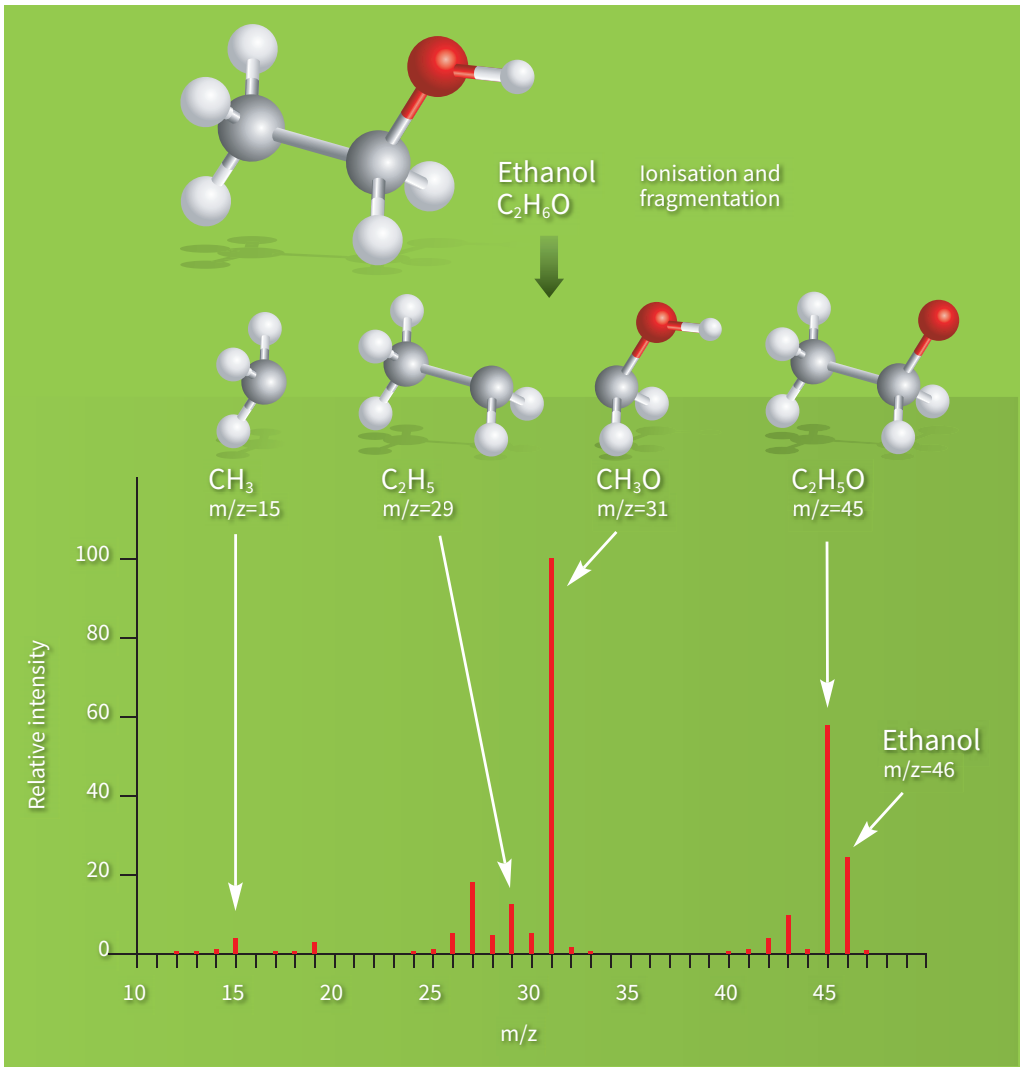
The high-energy electron bombardment may also cause molecules to be broken into many different fragments. For example, methane molecules (CH_4) can be fragmented to produce CH_3^+, CH_2^+, CH^+ and C^+.

The positive ions are then accelerated by an electric field and focused into a fine beam by passing through a series of slits with increasing negative potential. The beam of fast-moving positive ions is deflected by a strong external magnetic field.

The magnitude of deflection depends upon two factors, which are combined into the m/z ratio. When m/z is small, the deflection is large.

Finally, ions which make it right through the machine are detected electronically. As the positive ions arrive at the detector they pick up electrons to become neutral. This movement of electrons is detected, amplified and recorded. The external magnetic field involved in deflection can be adjusted so that ions with different m/z ratios can be detected.

A printout of intensity vs m/z ratio is produced. As the molecule gets bigger the possibility of fragmentation increases and the mass spectra become more complex. Final decisions about structure are made after combining evidence from mass spectroscopy with other analytical tools such as IR, UV and NMR.



The mass spectrum and resulting fragmentation pattern of ethanol (C_2H_6O or CH_3CH_2OH)

Modern mass spectrometry (MS) techniques

Liquid or gas chromatography combined with MS (LC-MS or GC-MS)

The techniques LC-MS and GC-MS are carried out in labs all over the world. They combine the separation technique of chromatography with the identification technique of mass spectrometry, to 'see' what a complex mixture is made up of.

The mixtures are first separated by liquid or gas chromatography. These techniques work in the same way as paper chromatography, in that a they exploit the affinity of a substance for one material over another in order to separate them.

In both gas and liquid chromatography, the substance is moved through a stationary phase in a fluid called the mobile phase. As the separated substances leave the column, they are automatically fed into a mass spectrometer so that each component of the mixture can be identified. Industries that use LC-MS and GC-MS include:

- proteomics – the study of proteins including digestion products;
- pharmaceutics – drug development, identification of drugs and drug metabolites – remember the Olympics and the drug testing of competitors;
- environmental – detection and analysis of herbicides and pesticides and their residues in foodstuffs.

High-performance liquid chromatography (HPLC) is a common technique used in analysis laboratories

High resolution mass spectrometry (HR-MS)

HR-MS can distinguish between compounds with the same nominal mass but different actual mass caused by their different elemental compositions. For example, C_2H_6, CH_2O and NO all have a nominal mass of 30, but their exact masses are 30.04695039, 30.01056487 and 29.99798882, respectively.

These subtle differences can be distinguished by this high-resolution technique. It is becoming increasingly important as a technique for analysing the interactions between drugs and body tissues at the scale of DNA.

Project 1

Observation and inference

Emission competition

- Themed lesson guide for teachers
- Teacher's project guide
- Class project instructions
- Student project portfolio

THEMED LESSON GUIDE FOR TEACHERS

Emission competition

Focus: **observation and inference**. Two–three lesson plan

1

This is a collection of lesson ideas to support students as they explore and develop their thoughts and skills in analytical chemistry. Through a flame test experiment and building a DIY spectrometer, students will get to consider the actual observation of scientific phenomena and compare it with the scientific skill of drawing conclusions based on data.

This project contains:

- a teacher-led practical;
- a student introduction to spectroscopy via a DIY spectroscope activity;
- a competitive student project based on carrying out flame tests which finishes with a photography competition to further enhance the 'observation' theme.

The first lesson opens with the inspiring story of an Irish teenager who won the Google Science Fair prize, which involved building his own spectrometer.

The section is fully supported by a PowerPoint presentation which guides the discussion to focus on the collection of data, asking the questions: 'What are the different ways in which scientists achieve this?' and 'What is the best way to present it?' Both questions feed into the photography competition.

Learning objectives

On completion of the project students will:

- be able to recall why scientists collect data, explain what an experimental observation is, and discuss the difference between observation and inference;
- have constructed a model spectroscope which will generate observable phenomenon;
- be able to carry out flame tests and have participated in a photography competition based on what they observed while carrying out their tests.

Pre-planning

- Collect some prizes for the winning photographs.
- Consider how you would like to receive the photographs – students could submit photos by email, or produce poster presentations.
- Consider printing and framing the winning entries to encourage future and current students.

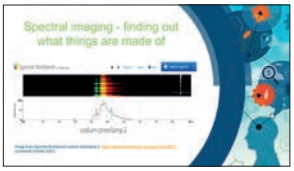
General equipment

- Black A4 card (alternatively colour white card black with permanent marker)
- Print-outs of the spectroscope template (found in the student explanation section)
- Craft equipment, a selection of coloured paper, cardboard and cellotape
- Flame test salts and equipment – Li, Na, K, Ba, Sr, $CuCl_2$

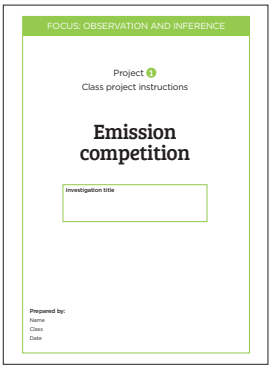
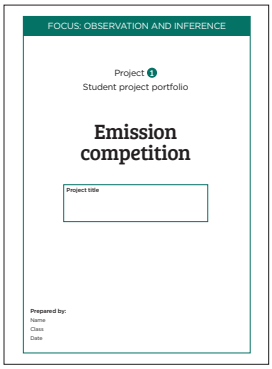
Additional resources

- For use with the suggested lesson plan PowerPoints, the **teacher's project guide**, the **class project instructions** and the **student project portfolio**.
- Visit **rsc.org/resources/analysis** for information and resources for teaching about spectroscopy **edu.rsc.org/resources/make-your-own-spectroscope/1289.article** and **edu.rsc.org/resources/flame-tests-using-metal-salts/1875.article**
- *The Nature of Science: Black Box*, or **edu.rsc.org/practical/identifying-ions-practical-videos-14-16-students/4011491.article**, **edu.rsc.org/resources/black-box/1275.article**

EMISSION COMPETITION: LESSON ONE
Recording results

STAGE/PURPOSE	RUNNING NOTES
Engage Get students interested in the idea of recording information.	 Display slide 2 shows the question, which introduces the themes of data collection and instrumentation.  Display slide 3 – students could discuss in pairs or as a group the answers to the questions on the board.
Scientific method This activity allows teachers to introduce key concepts for undertaking the scientific method. Including the focus for this project: observation and inference.	**Slide 3 – suggested activity** One of the most basic skills in scientific inquiry is the ability to make observations during experimental work. Students will often say what they think is happening rather than what they observe, eg stating that hydrogen gas is given off is not an observation in the true sense, because the student cannot see that it is hydrogen gas, and a further test would need to be carried out to verify this. A true observation would be 'a gas is given off'. **1** Students can be put into groups of two. **2** One student is given a picture, but they are not allowed to say what it is, only to describe it. **3** The partner tries to recreate the image by sketching it onto a piece of paper. **4** Students can then compare the picture with the sketch. **5** This will allow students to recognise their strengths in making observations and also communicating these observations, as well as improvements they would need to make in order to allow their partner to produce more accurate sketches. **6** The roles could then be reversed using a different picture, to allow the second student to make and communicate their observations.
Real world and careers link Get students interested in how this links to their career aspirations and industry in Ireland.	  Display slide 4 and 5 show how this is relevant to the real and global world. The link below outlines Finn's experiment, including details of his spectrometer (after several prototypes). Note: he makes a spectrometer and this project asks for a spectroscope – the former being quantitative and the latter qualitative. See **blog.google/outreach-initiatives/education/2019-google-science-fair-winners** for more details.  Display slide 6 shows condensed personalised versions of two careers stories (the full versions of which can be found in the **careers and industry** section).
Project and homework instructions	 Display slide 7 – discuss the photograph competition as a way to collect and present results. Give students the **class project instructions** sheets, and instruct them to follow along in their student **project portfolio** – shown overleaf. Give class time to make a basic spectrometer, and set as a homework to improve their model so that they can take the best picture.

EMISSION COMPETITION: LESSON TWO
Carrying out the investigation and write-up

STAGE/PURPOSE	RUNNING NOTES
Flame test Giving students the opportunity to conduct the experiment with their equipment.	Encourage the students to use the vocabulary of observation and inference and allow them to write up the results in the **student project portfolio**. They should be encouraged to finish the write-up at home and to submit photos for the photo competition – perhaps sharing the categories with the students in advance.  

EMISSION COMPETITION: LESSON THREE
Presentation and prizes

STAGE/PURPOSE	RUNNING NOTES
Presentation	Discussing with the students the merit of the pictures encourages a culture of evaluation.

Suggested photo categories

1. Best picture
2. Most original (source of light)
3. Best instrument
4. Best explanation of emission spectrum
5. Best variety of photos

Useful links

1. **solar-center.stanford.edu/activities/cots.html**
2. **livescience.com/41548-spectroscopy-science-fair-project.html**
3. **exploratorium.edu/snacks/cd-spectroscope**

Project 1

Teacher's project guide

Emission competition

Finding out what things are made of

Prepared by:

Name

Class

Date

EMISSION COMPETITION
Planning sheet

Why are you doing this investigation?

What do you want to find out? This could be some type of hypothesis or idea you want to prove or disprove, or a way to explain a complex process.

Include any inspiration for undertaking the project. This could be some type of hypothesis or idea you want to prove or disprove, or a way to explain a complex process.

What do you think you might discover or find? This could be some type of hypothesis or idea you want to prove or disprove, or a way to explain a complex process.

Flame test variables

Students should identify that the salt will be the independent variable, the flame colour the dependent and that the 'results' will be the thing they have determined, or inferred. To support this, students should be given a copy of the metal ions and their corresponding colours, or alternatively research them. Here is a useful resource using the wooden splint method **edu.rsc.org/resources/flame-tests-the-wooden-splint-method/759.article**

1

Deciding on your method and instrument

It is good to encourage the students to focus on how they will record the evidence. This will allow students to imagine which version of the spectroscope they are most interested in creating – a high-tech or low-tech one. They need to think about how they will attach the camera, as the quality of recording materials will affect the quality of the observations.

Suggestion for attaching a phone

You can find detailed guidance on how to build a smartphone spectrometer and record emission spectra in this resource **edu.rsc.org/download?ac=15353**

This design from Public Lab gives also advice on how to analyse the spectra using Spectralworkbench **spectralworkbench.org**

Discussion

A discussion could be started about how the camera might provide less biased answers than relying on humans. However, it should also be pointed out at some stage that cameras tend to have filters and also that pictures can be altered before and after printing. Which is more reliable? People or cameras? Or both?

EMISSION COMPETITION
Results

When recording results scientists normally collect quantitative data, which is usually in the form of numerical values, like concentration or wavelength. Then they use this to carry out calculations or present the values in a graph to establish a relationship between independent and dependent variables.

For qualitative data, observational data is usually collected and inferences made based on the work of previous scientists.

Table of results

OBSERVATIONS		
Salt to be tested	**Colour of flame**	**Corresponding metal ion**
A	Magenta	Li
B	Yellow	Na
C	Lilac	K
D	Yellow-green	Ba
E	Crimson-red	Sr
F	Blue or green	Cu

Students should be clear these are qualitative and that to make it quantative they would need to add numbers, eg wavelength.

Supportive results

This would include photographic evidence of your results.

Suggested categories

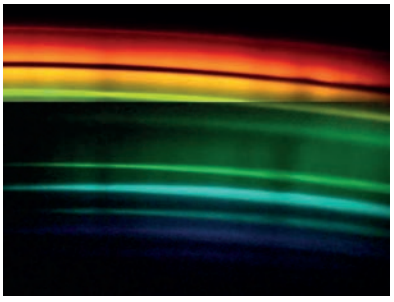
1 Best picture

2 Most original (source of light)

3 Best instrument

4 Best explanation of emission spectrum

5 Best variety of photos



High-pressure sodium light and its spectrum

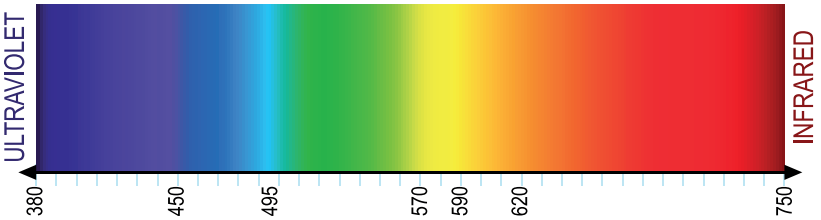
EMISSION COMPETITION
Analysis and conclusion

In this section they should describe which salt is which and explain using their observations, eg I believe salt one is a sodium salt because it produced a bright orange flame.

Inference **Observation**

They should support this inference or deduction by referring to well-known scientific facts, eg that sodium produces a bright orange light when heated.

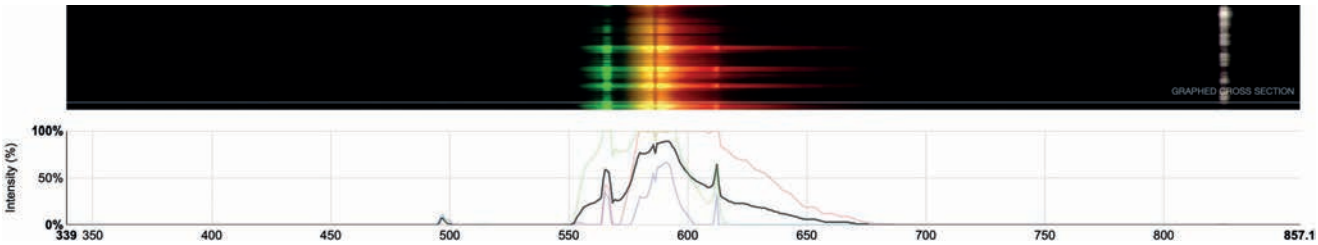
Some will go further and use the wavelength as a quantitative reference, if they had a calibrated spectrometer, eg 'I believe the salt was sodium based on the peak at 590 nm'.



The emission spectra with corresponding wavelengths

An example is included below, taken from Spectral Workbench **spectralworkbench.org**

This document explains how to analyse these spectra **edu.rsc.org/download?ac=15350**



Emission spectrum from a sodium street lamp

Project 1

Class project instructions

Emission competition

Investigation title

Prepared by:

Name

Class

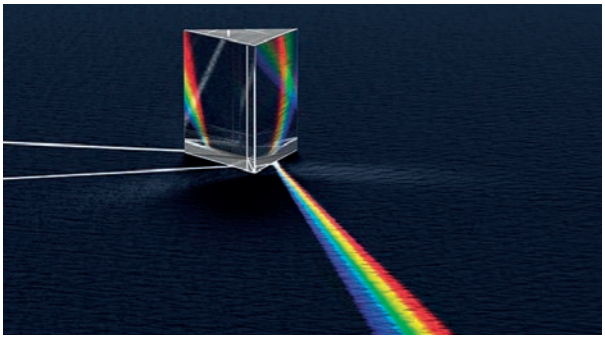
Date

CLASS PROJECT INSTRUCTIONS
Finding out what things are made of

1

Background

The first spectroscopes were prisms with graduations credited to Gustav Robert Kirchoff and Robert Wilhem Bunsen. They evolved to include a slit for the light and a lens to narrow the beam. The spectroscope quickly became valued for its ability to measure the wavelength and the intensity of light.[1]



Using prisms as early spectroscopes

Kirchhoff, like many other scientists at the time, was beginning to unravel the secrets of light. He discovered that the bright lines he saw in his spectroscope were the same pattern of dark lines he found when he looked at the sun, and he realised this was absorption and emission of some kind, concluding that this could only mean one thing – that the sun and the stars were made of the same things as here on Earth.

The pattern seen in the spectroscope[2]

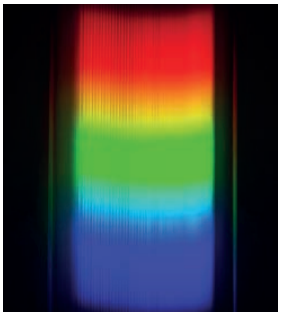
So he and Bunsen began, like many students do, putting whatever 'elements' they thought they had into the Bunsen flame and watching the different spectra lines. They concluded – as you will too – that each pattern represents a different substance. In this method Kirchhoff had discovered an exquisite analytical method, capable of identifying elements.

Different light sources

Many light sources exhibit different forms of the spectra. Look at the two below.

The sun and many torches emit all the colours of the rainbow and a continuous spectrum of all the colours can be seen.[3]

If you look at a TV screen or a fluorescent light you will see separate lines of different colours.[4]



The spectra seen when looking at the sun[4]

The spectra seen when looking at the TV [4]

Missing or extra light tells us that certain elements have been affected. Astronomers and chemists study these spectra because they contain information about the light source.

This is particularly useful when working out the composition of distant stars and indeed was used to discover the composition of our own sun.

Some spectra of individual elements[2]

Hydrogen absorption spectrum

Helium emission

Hydrogen emission spectrum

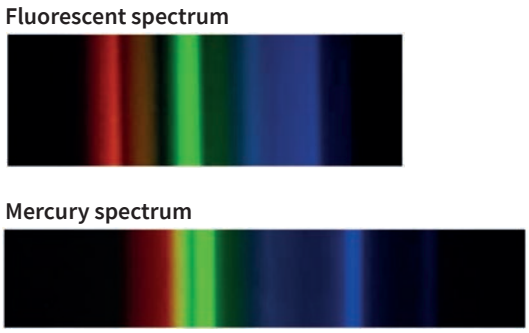
References

1 **sciencehistory.org/historical-profile/robert-bunsen-and-gustav-kirchhoff**
2 Free resources available at **solar-center.stanford.edu/activities/cots.html**.
3 **chemistryworld.com/opinion/kirchhoffs-spectroscope/6547.article**
4 **edu.rsc.org/resources/make-your-own-spectroscope/1289.article**

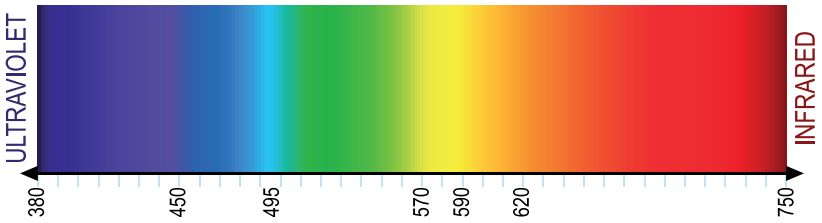
Comparing a pure sample and a mixture

Composition can also be determined by comparing a sample with pure spectra. This is shown on the right, where the lines in the photo of fluorescent light correspond to the lines shown in pure elemental mercury, proving that fluorescent light contains mercury.

Another more accurate way to describe this overlap is to describe the light in terms of its wavelength and often its intensity, shown below.



Comparing a sample with pure spectra[2]



The emission spectra with corresponding wavelengths

Scientists use instruments all the time and through this project you will build your own. This will give you a keen insight into why instruments are so important, what you should be looking for and also the best ways to record and interpret your results.

Your task

Your task is to find out what metals are present in the salts using a combination of flame tests and emission spectroscopy and to record and present your results. You can take photo's of each metal's emission spectrum. But first you will need to build your instrument!

Making your spectroscope

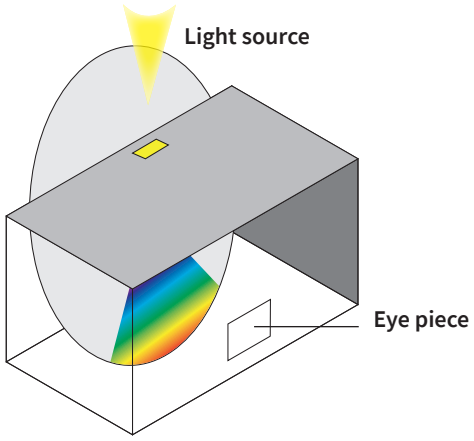
The simplest spectroscope can be created using the template provided and a CD.

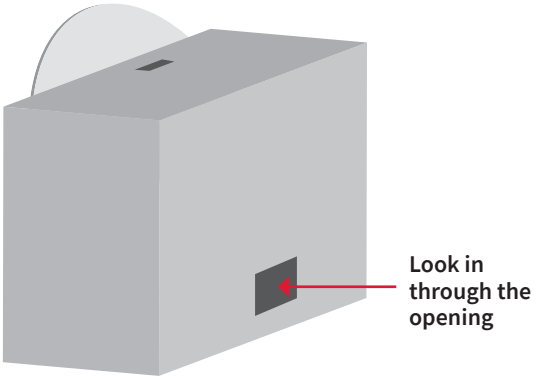
The end product is shown in the image – it is advisable to tape down the CD so it doesn't wobble, while you look through the eye piece.

However, there are a number of different types and designs, so choose wisely!

Hint! There are many YouTube videos demonstrating how you can make a simple spectrometer and take pictures using a phone camera. Here is one from MIT OpenCourseWare **youtube.com/watch?v=fl42pnUbCCA**

How it works





The completed spectroscope – see template provided overleaf

1

2

3

Make your own spectroscope

1 Glue this template onto an A4 piece of card.

2 Cut along all the solid black lines with scissors, including line **a**, and cut out the rectangles **b** and **c** (it's a bit tricky!).

3 Fold along all the dotted black lines.

4 Make the template into a box by joining the same numbered flaps together, eg **1** joins to **1**.

a

b

5 Put a CD into the box through the slot you made at line **a** with the bottom 'rainbowy' side of the CD facing upwards.

6 Look into the box through the square hole and you should be able to see light split into a rainbow.

7 Try looking at different types and colours of light and see what changes in your spectroscope.

2

3

c

1

EMISSION COMPETITION
Planning sheet

Why are you doing this investigation?

What do you want to find out? This could be some type of hypothesis or idea you want to prove or disprove, or a way to explain a complex process.

Include any inspiration for undertaking the project. The work of other scientists (particularly anything from the careers stories), or things in the media that might have motivated your interest in this topic.

What do you think you might discover or find? This should link to the focus of research and analysis – how your results will prove or disprove your hypothesis or idea.

Flame test variables

You will test six different salts, make an observation and from these you will determine their identity. In your group identify which variable is which:

Corresponding salt	**Independent variable** – the thing you change each time.
The colour of the flame	**Dependent variable** – the thing you measure, which changes depending on the independent variable.
Salt to be tested	**Results** – the thing you have determined.

Deciding your method and instrument

To record your observations, you should first be clear on what an observation can be, ie something you can: see; feel (heating up or cooling down); hear; smell.

These are things you cannot easily determine, for example, 'things fall because of gravity'. This is something you have understood to be true but did not determine in the experiment. The correct observation could be 'unsupported things fall to the ground'. This is the difference between observation and inference.

Once you have built your own spectrometer, you can use it and your smart phone to take photo's of the emission spectrum of the flame produced by each metal salt. You could use any free light meter app available on your smartphone to make a measurement.

Include a description of how you will collect your observations. Hint! diagrams are helpful

EMISSION COMPETITION
Results

When recording results scientists normally collect quantitative data, which is usually in the form of numerical values, like concentration or wavelength. Then they use this to carry out calculations or present the values in a graph to establish a relationship between independent and dependent variables.

For qualitative data, observational data is usually collected and inferences made based on the work of previous scientists.

Table of results

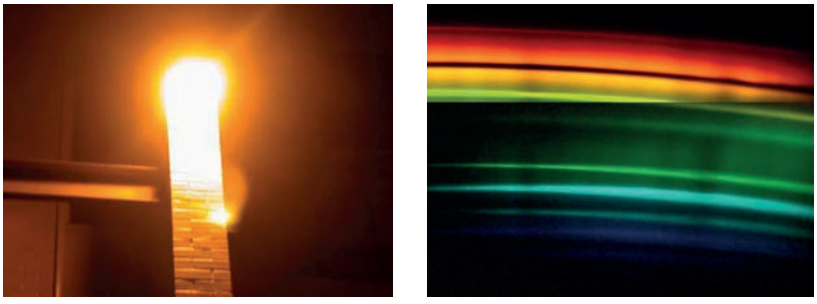
OBSERVATIONS		
Independent variable	**Dependent variable**	**Results**

Do you think these results are qualitative or quantative?

Supportive results

This would include photographic evidence of your results for the emission competition.

Your work should be presented with a photo of the light and a picture of its spectrum, eg see the sodium streetlight photos below.



High-pressure sodium light and its spectrum

This will be a competition to see who can produce the best photos – the emission competition.

Include a link or print out of your photos.

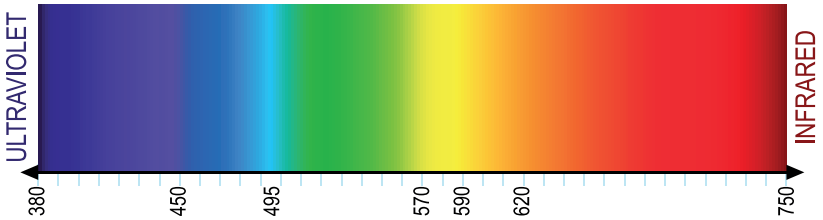
EMISSION COMPETITION
Analysis and conclusion

In this section they should describe which salt is which and explain using their observations, eg I believe salt one is a sodium salt because it produced a bright orange flame.

Inference **Observation**

They should support this inference or deduction by referring to well-known scientific facts, eg that sodium produces a bright orange light when heated.

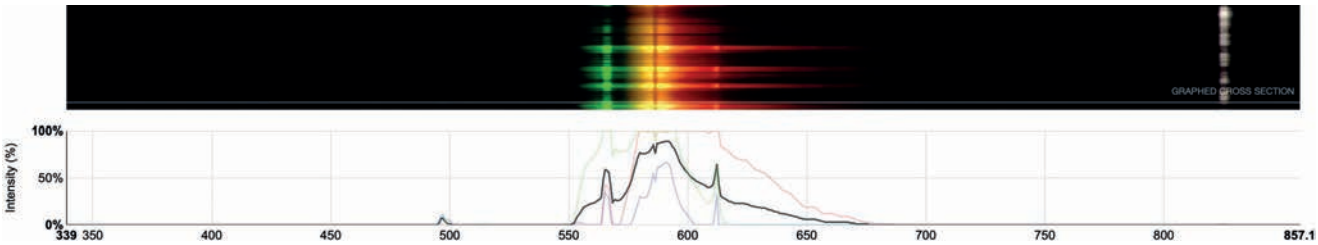
Some will go further and use the wavelength as a quantitative reference, if they had a calibrated spectrometer, eg 'I believe the salt was sodium based on the peak at 590 nm'.



The emission spectra with corresponding wavelengths

An example is included below, taken from Spectral Workbench **spectralworkbench.org**

This document explains how to analyse these spectra **edu.rsc.org/download?ac=15350**



Emission spectrum from a sodium street lamp

Project 1

Student project portfolio

Emission competition

Project title

Prepared by:

Name

Class

Date

EMISSION COMPETITION
Planning sheet

Why are you doing this investigation?

Variables

Deciding your method and instrument

Spectroscope diagram

1

Table of results

Emission competition

Explain your observations

Project 2

Accuracy and precision

Phone-y science

- Themed lesson guide for teachers
- Teacher's project guide
- Class project instructions
- Student project portfolio

THEMED LESSON GUIDE FOR TEACHERS

Phone-y science

Focus: **accuracy and precision**. Four–five lesson plan

2

Task

Using mobile phone devices and apps to collect colorimetry data.

Background

Computers have revolutionised science and its ability to capture and analyse data, and now smartphones are showing the same potential. Thanks to their evolving technology and growing use many of us now have easy access to sophisticated instrumentation.[1] Some current research is using smartphones for colorimetric water quality analysis, soil analysis and air quality. This, coupled with GPS, has the potential to influence pollution management and policy.[2]

The idea behind this project is to get students familiar with the idea of spectrometry and the type of laboratory equipment that can generate results. It is hoped that producing their own results with their own equipment will inculcate an increased appreciation for accuracy and precision, and thus how the design of a method and its robustness can infer more reliable data. It also engages them with the questions surrounding 'the reliability and potential for using mobile phones for data collection'.

Learning objectives

On completion of the project students will:

- have increased their familiarity with colorimetry and mobile devices as tools for data collection;
- be able to describe the scientific method, in particular the difference between accurate and precise;
- have applied their subject knowledge as part of analysing and presenting the results of their project;
- be able to describe the relationship between concentration and absorption.

Pre-planning

- Ideally, students will have completed the relevant sections in this booklet before attempting the project to support their learning. They should have a basic understanding of accuracy and precision, how to draw and interpret graphs and colorimetry.
- Because the app charges a small fee it is advisable that at least one person in each group downloads this in advance, as usually children need permission from their parents to complete these payments.
- Prepare different coloured solutions of known concentrations and have different coloured paper for the investigation stage.

General equipment

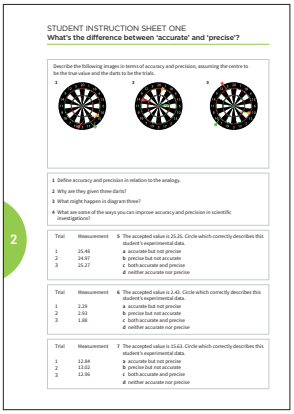
- Blackcurrant or other similar juice, or any coloured standard solutions.
- Colorimeter app, colorimeter lab equipment if possible to check real values.
- Craft equipment, a selection of coloured paper, cardboard and cellotape.

Additional resources

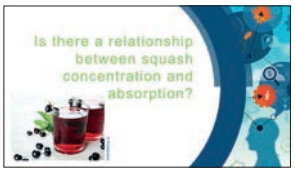
- For use with the suggested lesson plan PowerPoints, the **teacher's project guide**, the **class project instructions** and the **student project portfolio**.
- Visit **edu.rsc.org/resources/analysis** for information and resources for teaching about spectroscopy.
- Video demonstration and resource **edu.rsc.org/resources/smartphone-spectroscopy-changing-concentrations/4012061.article**

References
1 McGonigle *et al*, Sensors, 2018, **18**, 223.
2 C Sicard *et al*, Water Res., 2015, **70**:360-9.

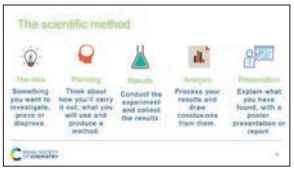
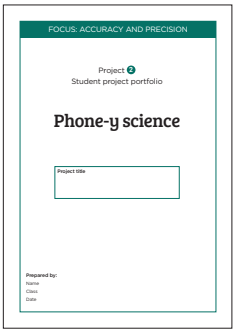
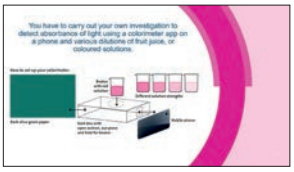
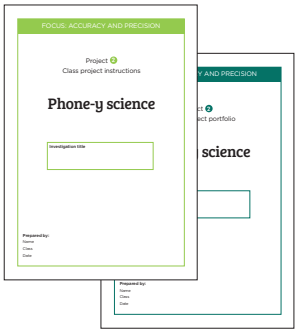
PHONE-Y SCIENCE: LESSON ONE
The difference between accuracy and precision

STAGE/PURPOSE	RUNNING NOTES
Engage Get students interested in instrumentation and how they can become a part of it, while asking if the data generated is actually reliable.	 Display slide 2 shows the question to facilitate discussion and open up the themes of data collection and instrumentation.  Using slide 3, students could discuss in pairs or as a group, the answers to the questions on the board.
Real world and careers link Get students interested in how this links to their career aspirations and industry in Ireland.	  Display slides 4 and 5 give global context to show how this is relevant to the real world.   Display slides 6 and 7 show condensed personalised versions of two careers stories.
Scientific method This section allows teachers to introduce key concepts for undertaking of the scientific method.	    Slides 8, 9 and 10 focus on the concept of accuracy and precision. This could be completed with an actual dartboard or using the subsequent slides to discuss the differences in the concepts. The PowerPoint should be used in conjunction with **student instruction sheet one**. Further discussion points include: • the importance of carrying out at least three trials in order to gain more accurate results; • anomalous results; • repeating experiments until you get concordant results; • using averages to get more accurate values to use in calculations; • more accurate and less accurate glassware in analytical chemistry; • instrumentation as a way to improve accuracy and precision; • systematic errors such as consistently reading the burette wrong; • the importance of methods and techniques to reduce errors such as reading the meniscus from the bottom each time instead of the top.

2

STAGE/PURPOSE	RUNNING NOTES
Pre-project knowledge Colorimetry-1 Skip this if you are confident students understand the relationship between absorption and concentration.	 Present slide 11 using the following teaching strategy: → 10 students lined up in front of the room. → Five students are wearing the same coloured sticker. Each student represents a particle of the substance. → The remaining five students represent the solvent the substance is dissolved in; these students stand with their hands behind their back. **1** Turn a light on to indicate the start of the simulation and then release 10 white balls (scrunched up pieces of paper will work just the same). **2** Only students wearing a sticker can lift one ball. **3** Five balls are lifted, therefore five remain. Students can see if we know the 'amount' of light initially used, we can see how much was absorbed and how much passed through. Allow students to begin to understand how absorption of light can be used to form a relationship with the concentration of substances in a solution.
Colorimetry-2 Help students to understand and distinguish between the colour of light being absorbed and measured versus the colour of the solution.	Define colorimetry for the class. You can use the following extension on the teaching strategy above as a means to consolidate your student's understanding of the topic. To allow student's to visualise this concept: **4** The same students are selected again, each wearing the same coloured sticker. This time two (complimentary) coloured balls are thrown at the students (eg blue and orange). Each student is only allowed to catch a matching coloured ball to their sticker. Ask students to put the matching coloured ball in their pocket or out of sight of the rest of the class. This represents the colour that has been 'absorbed' and is what will be 'measured' in the experiment. The ball that was not caught, will fall to the floor, this represents the colour of the solution that we will see. This is a visual illustration of the absorption of certain wavelengths of light in a solution. 

PHONE-Y SCIENCE: LESSON TWO
Planning the project and carrying out the investigation

STAGE/PURPOSE	RUNNING NOTES
Project introduction and criteria Giving an overview of the project and the scientific method.	  Display slide 12 shows the key stages of the scientific method. These overlap with key sections in the **student project portfolio**.
Project instructions and investigation Students should be encouraged to play around with the equipment before deciding on a method and collecting results.	  Display slide 13. **1** Put students in groups and give each group a copy of the **class project instruction** sheets. **2** Give each student a copy of the blank **student project portfolio** sheets. **3** Allow them to plan and investigate which method they will choose. During this section students should be able to explore the best method for their investigation. This will require some setting up of equipment, use of craft materials and the coloured solutions. Finally, when the group is clear about their method, give each student a blank **student project portfolio**. Ask them to individually fill in the planning section of the report and collect their data.

PHONE-Y SCIENCE: LESSON THREE
Analysis

STAGE/PURPOSE	RUNNING NOTES
Project analysis This stage will allow students to apply their knowledge of colorimetry and explain the intricacies of accuracy and precision.	Drawing graph and completing results analysis. → The **class project instructions** contain comprehensive help with how to conduct this analysis. Students should be given the real values for concentration of solutions and allowed to compare them, or be shown how to calculate this (see the **teacher's project guide** for method). **Extension task** – they also must compare their results with another group to ascertain the difference with respect to the instrument or method. Alternatively, they could collect results using different solutions. Begin preparing the presentation – class time could be given for this and additional time as a homework. They should be given access to the **careers and industry stories** to be used in their presentations.

2

STAGE/PURPOSE	RUNNING NOTES
Presentation Consolidate and demonstrate knowledge acquisition. Peer marking – allows the students to evaluate the work of others.	Students could be given a lesson to prepare their presentations or it could be set as a homework task. To encourage the students to evaluate the work of others, and noticing the different ways of conducting the same experiment, showing their method and how this fits in with the research. See instructions and a marking rubric below.

Presentations: three–four minutes long

- A brief overview of what you did, including what was unique about your method and explaining why you chose to do it that way.
- What went well and what could have been improved.
- How your results compared to the real values for the stock solutions or another groups, and which you thought was more accurate/precise and why.
- Talk about how this relates to analytical chemistry and instrumentation in the real world.
- Focusing on one careers story, describe how the use of smartphone technology could (in the future) make the role of the scientist more effective – imagination is encouraged.

Marking rubric

TASK	EXCELLENT	GOOD	MISSING	COMMENT
Introduced the investigation				
Their design				
Why they chose it				
What went well etc				
Did they compare results?				
Did they explain correctly who was more accurate or precise and why?				
Did they talk about how this related to the chemistry in industry?				
Career story focus?				

Project 2

Teacher's project guide

Phone-y science

Investigating how mobile phone devices and apps can be used to collect colorimetry data

Why are you doing this investigation?

What do you want to find out? If phones can be used to produce reliable data, ie values that resemble the true concentration.

Include any inspiration for undertaking the project. The work of other scientists, such as those in the careers portfolio, or those projects mentioned in the background information.

What you think you might discover or find? If mobiles can be used to collect accuracy or precise data, and this could be relied on by scientists.

Deciding your method

Students should be encouraged to undertake this as a team, being more creative than the diagram given. This set up is-simple, but many variations are possible and the students should be encouraged to explore their own method with repeatability and accuracy as the main goals. Discuss drawbacks, for example, it has no infrastructure for holding the phone in place.

For your own guidance, you can watch a video by the Royal Society of Chemistry education coordinator in Ireland **edu.rsc.org/resources/smartphone-spectroscopy-beer-lambert-law/4013028.article**

Additional useful resources on the topic:

- Science in School's secondary school teacher's resource **scienceinschool.org/content/smartphones-lab-how-deep-your-blue**
- Professor of chemistry, Tom Kuntzleman's blogpost and video **chemedx.org/blog/use-your-smartphone-absorption-spectrophotometer**

Variables

Students should be encouraged to identify their own variables and design in how they will encourage precision and accuracy.

Here are some exercises you can use to demonstrate these concepts:
edu.rsc.org/cpd/making-measurements/3009329.article
edu.rsc.org/lesson-plans/accuracy-and-precision-in-practical-investigations-14-16-years/108.article

Independent variable – concentration or dilution of the juice/solution

Dependent variable – the RGB (red, green and blue) value given by the phone on the colorimeter app. They will need a blank, and at least three trials.

Higher level (HL) students could be selected to decide and create the class dilutions – it's better to have class dilutions or a few sets so that accuracy and precision and instrumentation can be compared.

Raw data

Blank	182
	168
	180
Dilution 1	25
	17
	26
Dilution 2	65
	85
	68
Dilution 3	119
	98
	136
Dilution 4	150
	153
	161

Averaged results table

Blank	176.67
Dilution 1	23.00
Dilution 2	72.67
Dilution 3	117.67
Dilution 4	154.67

Graph

Students plot a graph of absorbance against the dilution, calculating the absorption using the following equation:

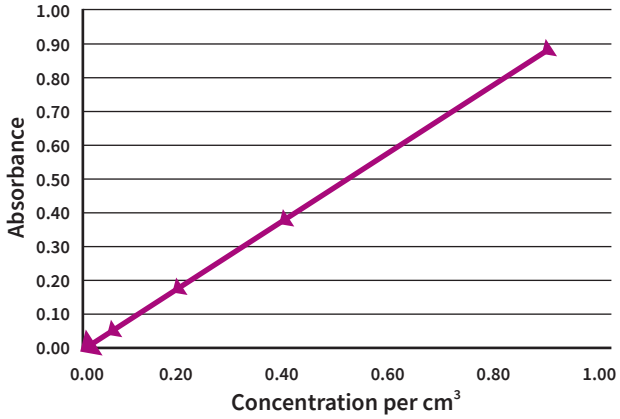
–log(G value/blank value)

Students could plot a graph of dilution 1, 2, 3, 4 or they could be encouraged to calculate the actual concentration, either by their own dilutions or the pre-arranged concentrations.

In this example, we used a bottle of strawberry juice, stating it was 5% juice. 5% v/v means that in 100 cm^3 there is 0.05 cm^3 of juiced strawberry.

Dilutions were made to stretch the range of colour graduation. Start with half or 50% dilution in the first instance, suggested dilutions are shown below. Students should convert their dilutions to a concentration using the units of volume they used for their dilution.

Concentration (cm^3)		Absorption
Blank	0.0000	0.00
Dilution 4	0.0030	0.06
Dilution 3	0.0060	0.18
Dilution 2	0.0125	0.39
Dilution 1	0.0300	0.89



Graph analysis

The line should be linear if it obeys Beer's Law, if not then it is likely that something went wrong in the method, eg moving the phone a different distance each time.

It is important to note that the equipment is not a colorimeter of laboratory sophistication, but enough to allow students to see the variability in equipment and method, while retaining the same technical operations as a colorimeter.

The student sheet has some comprehensive explanations for this section, including an estimate of what they should find. Ensure the answer matches the trend they found and also that they used their own values in the explanation.

Example: As concentration increases the absorbance of light at this wavelength is also increasing, eg a concentration of 0.0125 gives an absorbance value of 0.39 as the concentration was doubled to 0.03 the absorbance was also almost doubled 0.89.

These results would reflect what is to be expected, a higher concentration means more molecules, therefore there are more molecules absorbing the light, so the absorbance is higher at higher concentrations.

2

Conclusion

Uncontrolled variables

Distance would have affected this, as well as the transparency of the cup, the light in the room, the camera operator.

Accuracy and precision

Students should be encouraged to compare results with another group that had a similar set-up and solutions. Ideally, they could be compared with a class colorimeter, or the teacher's set of results.

Additionally, you could measure the RGB of the actual page – do this with the cup and compare the 'standard' values. For example, a photograph of the green page revealed the actually RGB 'G' value to be 255. The values for the blank were just above half of this.

Answers to student questions

1 Define accuracy and precision in this analogy. *Accuracy refers to how close a dart is to the bull's eye. Precision refers to how close the darts are to each other and is independent of accuracy.*

2 Why are they given three darts? *Trials.*

3 What might happen in diagram three? *They might generate an average of the three trials but this should be disregarded due to the imprecision.*

4 *Glassware, equipment, instrumentation, repeating trials.*

5 *A – accurate and precise*

6 *C – accurate and precise*

7 *B – precise but not accurate*

Scientists use standard procedures and calibration testing to reduce measurement errors.

Project 2

Class project instructions

Phone-y science

Investigation title

Prepared by:

Name

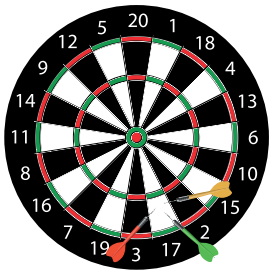
Class

Date

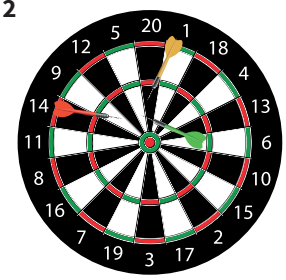
STUDENT INSTRUCTION SHEET ONE
What's the difference between 'accurate' and 'precise'?

Describe the following images in terms of accuracy and precision, assuming the centre to be the true value and the darts to be the trials.

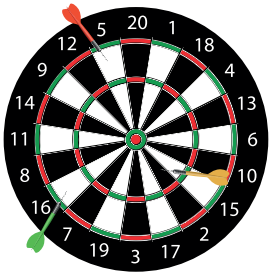
1



2



3



1 Define accuracy and precision in relation to the analogy.

2 Why are they given three darts?

3 What might happen in diagram three?

4 What are some of the ways you can improve accuracy and precision in scientific investigations?

2

Trial	Measurement
1	25.48
2	24.97
3	25.27

5 The accepted value is 25.35. Circle which correctly describes this student's experimental data.

a accurate but not precise
b precise but not accurate
c both accurate and precise
d neither accurate nor precise

Trial	Measurement
1	2.29
2	2.93
3	1.88

6 The accepted value is 2.43. Circle which correctly describes this student's experimental data.

a accurate but not precise
b precise but not accurate
c both accurate and precise
d neither accurate nor precise

Trial	Measurement
1	12.84
2	13.02
3	12.96

7 The accepted value is 15.63. Circle which correctly describes this student's experimental data.

a accurate but not precise
b precise but not accurate
c both accurate and precise
d neither accurate nor precise

STUDENT INSTRUCTION SHEET TWO

Using mobile phone devices and apps to collect colorimetry data

Background

Computers have revolutionised science and its ability to capture and analyse data, and now smartphones are showing the same potential. Thanks to their evolving technology and growing use many of us now have easy access to sophisticated instrumentation.[1] Current research uses smartphones for colorimetric water analysis, soil analysis and air quality analysis. This, coupled with GPS, has the potential to influence pollution management and policy.[2]

Your task

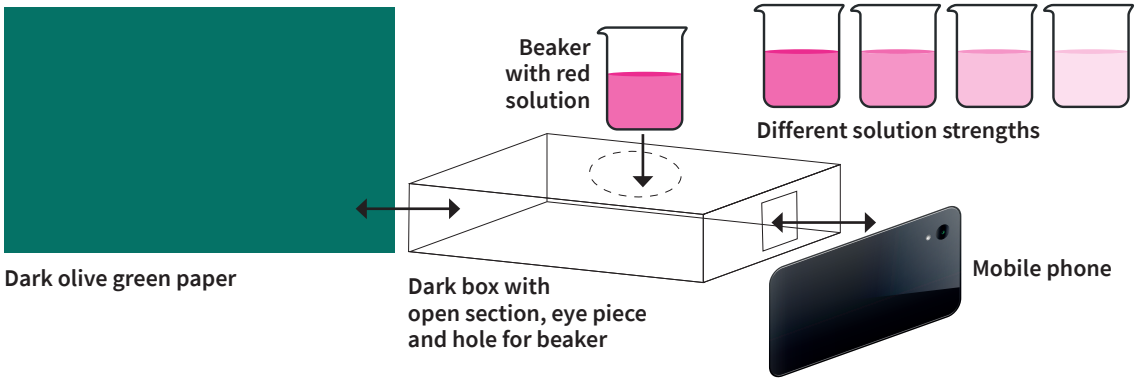
Your task

You have to carry out your own investigation to detect absorbance of light using a colorimeter app on a phone and various dilutions of fruit juice, or coloured solutions. It's a group activity and presentation but with an individual report. Hint! Look for videos and blogposts on the topic.

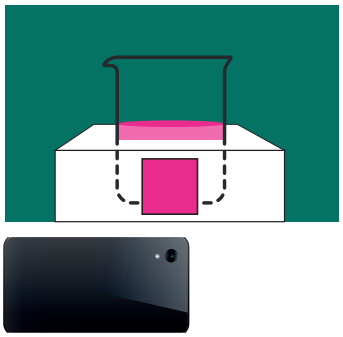
Task list per group

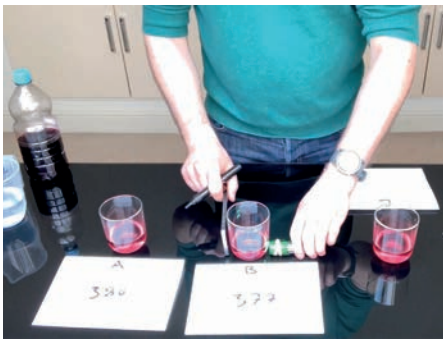
- ☑ Collect student project portfolio
- ☐ Download the app
- ☐ Collect equipment
- ☐ Investigate method
- ☐ Fill in portfolio
- ☐ Prepare presentation

How to set up your colorimeter



What it looks like from the phone





Using any free light meter application on your smartphone, you can collect and record the absorbance values of the coloured solution as shown in this video: **youtu.be/0954J_5NI88**

References
1 McGonigle *et al*, Sensors, 2018, **18**, 223.
2 C Sicard *et al*, Water Res., 2015, **70**:360-9.

Using mobile phone devices and apps to collect colorimetry data

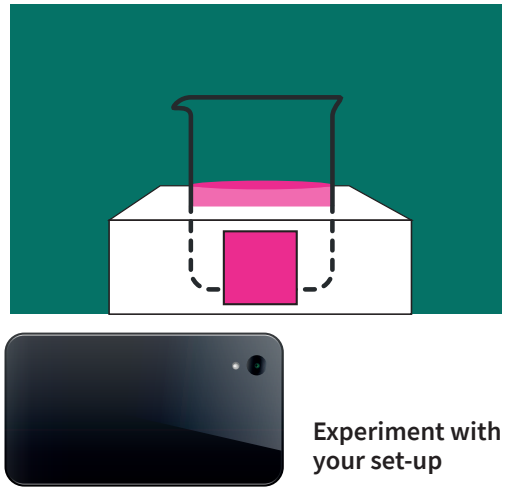
How it works

Your phone has some pretty sophisticated light and colour reading technology. You may have heard of RGB sensors – this means that red, green and blue light is measured by your camera in order to store the information from the photo as a picture.

By interrupting this light with different concentrations of solutions you can obtain a value for this 'interruption', which will vary much like the absorbance. If the solution is red then it's the green light we are most interested in so we will place a green page behind the juice.

To restrict the light passing through the solutions, we have placed it in a dark container, with a hole for the cup or beaker, an eye piece and an open section where the green light will be focused. This is an example set-up, and you are encouraged to trial different methods and set-ups to generate the most accurate results possible.

RGB colour recording



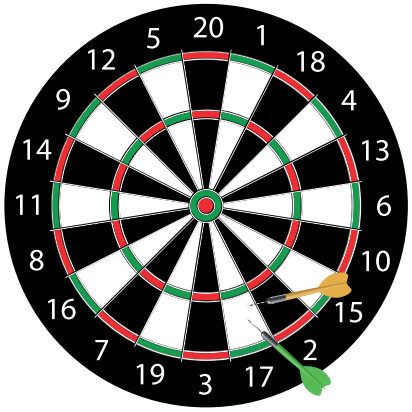
Experiment with your set-up

How will you know if they are accurate or not?

What can you compare them with?

Think about how you will improve your chances of getting the most correct value – this will probably relate to how much extra light you can restrict both in the box and with the distances between the light capture and your phone.

Investigate by changing a number of different variables before deciding on your method.



Accuracy and precision

Planning sheet

Why are you doing this investigation?

What do you want to find out? This could be some type of hypothesis or idea you want to prove or disprove.

Include any inspiration for undertaking the project, eg the work of other scientists, how using mobile phones and apps might improve quality of life for you or others.

What do you think you might discover or find? This should link to the focus of 'accuracy and precision'.

Deciding your method

Play around with the app and explore how the measurements change in response to different coloured liquids and pieces of paper.

What variables does the app measure and which ones are you responsible for changing?

Hint! Describe any two changes that you made in your experiment.

Variables

What are your project variables including control variables?

Are there any control variables that you will not be able to control, and what impact do you think this will have on your results?

Include a photograph or a diagram of your equipment set-up

For qualitative data, analysis of the data can usually be done from the table of results as this requires making observations and the inferences from the observations.

Raw data

This should be a table of results you collected, without any processing – that means it comes straight from the phone.

Help: Averages are used by scientists to get an even more accurate result. They allow for random variation and human error to be absorbed into the total – increasing the accuracy.

Averaged results table

You should average your three measurements for each dilution. This means add them all together and divide by three (if you carried out three trials).

You should then include a column for the absorbance, calculated using the equation below:

$$-\log(\text{G value}/\text{blank value})$$

For quantitative data, analysis involves collecting numerical values, using this to carry out calculations or presenting the numerical values in a graph to establish a relationship between independent and dependent variables or to find an unknown value.

Graph

Graphs should only be drawn from averaged results. You should plot absorbance against concentration.

Draw your graph by hand or on Excel and paste it in the box below.

2

Affix graph here

Marking criteria for the graph

- Axis drawn using a pencil and a ruler.
- Axis labelled with correct headings and includes units.
- An appropriate scale was used.
- Points plotted correctly.
- Line of best fit drawn.

Analysis and conclusion

Describe the relationship that has been established between the independent and dependent variables and link this back to the theory if possible.

Checklist for analysing the graph

1 **Make a statement describing what the graph shows**, eg 'As the concentration of the standard solution increases, the absorbance of light changes.'

2 **Establish the relationship between the independent and dependant variable**, eg concentration and absorbance are linked. As concentration increases, the absorbance of light at this wavelength is also increasing.

3 **Use the results, usually two as evidence**, eg when the concentration was 1 ppm the absorbance was 0.5, when the concentration of the standard solution was 5 ppm the absorbance was …

HL 4 Link this to the theory explaining why this relationship exists, state whether the hypothesis or question posed at the beginning of the investigation is correct, eg these results would reflect what is to be expected, a higher concentration means more molecules, therefore there are more molecules absorbing the light, so the absorbance is higher at higher concentrations.

Conclusion

How could you improve your results next time?

Reference accuracy and precision in your method and analysis to get more marks.

Make a concluding statement based on the accuracy and precision of your results. Also state what you have learned from the project, commenting on whether you think phones should be used to collect scientific data.

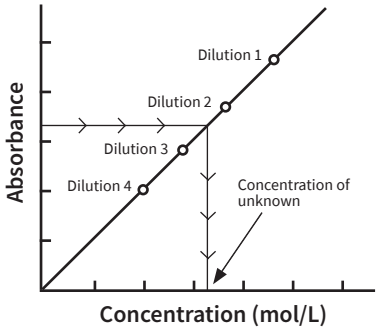
Thinking and research questions

How could your methods be applied to a real-life situation or used in industry? Also what would you need to change to achieve this?

How to draw graphs

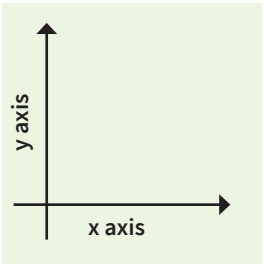
Colorimetry is a technique that relies on measuring the absorbance of a specific colour of light by a coloured solution and using this to work out the concentration of the analyte present.

The amount of light absorbed will be more or less, depending on the concentration. This technique allows us to work out the concentration of an unknown by placing on a scale along side known concentrations.



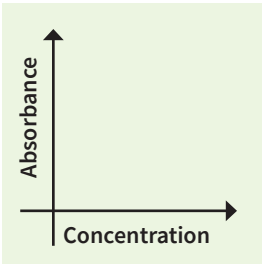
Colorimetry graph

1 Draw your axis using a ruler and a pencil



Hint! y is high, or 'wise up' (y's up)

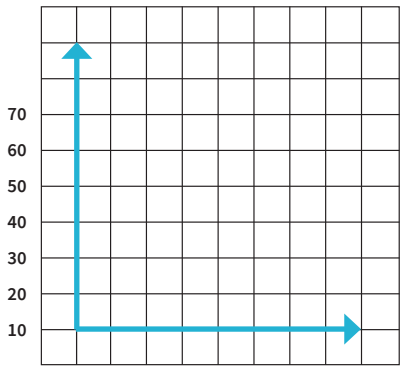
2 Label each axis with the correcting heading and include units where necessary



The dependent variable (what you measured) always goes on the y-axis.

The independent variable (what you altered) always goes on the x-axis.

3 Choose a suitable scale



Evenly spaced lines, eg with a value of 10 each

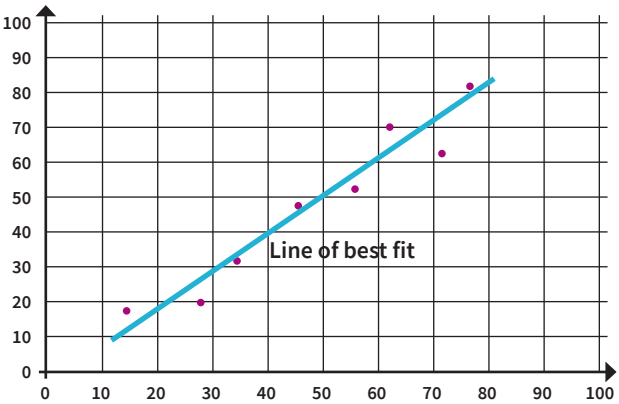
The scale you choose should allow all the results you require to be plotted. The scale should be evenly spaced and incorporate at least 75% of the graph paper so results can be clearly seen.

4 Plot your points accurately

Plotting points needs to be done carefully and accurately.

It is always wise to use a sharp pencil.

5 Draw your line of best fit



How to draw a line of best fit

Drawing a line of best fit can be difficult. It can be best described as a line that runs as close to as many points as possible. A good trick for this is to place your ruler on its thinnest side and try to get half the points on one side and half on the other. Then place it flat and mark your line.

Success criteria for good graphs

- Use a pencil and a ruler.
- Label axis with correct heading and units.
- Choose an appropriate scale.
- Plot your points accurately.
- Draw a line of best fit.

Project 2

Student project portfolio

Phone-y science

Project title

Prepared by:

Name

Class

Date

PHONE-Y SCIENCE
Planning sheet

Why are you doing this investigation?

Deciding your method

Variables

Include a photograph or a diagram of your equipment set-up

2

Results

Raw data

Averaged results table

Graph

Affix graph here

Marking criteria for the graph

- Axis drawn using a pencil and a ruler.
- Axis labelled with correct headings and includes units.
- Appropriate scale used.
- Points plotted correctly.
- Line of best fit drawn.

Graph analysis

Conclusion

Thinking and research questions

Project 3

Evaluating a scientific model

Building a mass spectrometer

- Themed lesson guide for teachers
- Teacher's project guide
- Class project instructions
- Student project portfolio

THEMED LESSON GUIDE FOR TEACHERS

Building a mass spectrometer

Focus: **evaluating a model**. Two–three lesson plan

3

Task

Building and using a model of a mass spectrometer and evaluating its utility.

Background

Mass spectrometry is a key technique in almost every laboratory analysis – this is profiled in the careers and industries stories. This project seeks to introduce students to the 'scientific model' by way of a model mass spectrometer, instilling an understanding of how it works and the type of data it generates, showcasing the use of models in general. To complete the project, students must engage with the data in a manner fitting of a scientific investigation, with the focus being evaluation.

Syllabus link

On completion of the project students will be familiar with:

- use of the mass spectrometer in determining relative atomic mass;
- calculating relative atomic mass from abundances of isotopes;
- fundamental processes that occur in a mass spectrometer – vaporisation of substance, production of positive ions, acceleration, separation, detection (mathematical treatment excluded).

Learning objectives

On completion of the project students will:

- have a basic understanding of how a mass spectrometer works;
- understand the scientific method, in particular the aspects of scientific modelling;
- be able to calculate the relative atomic abundance of different isotopes from graphical data.

Pre-planning

- Ideally, students will have completed the previous projects and gained a solid understanding of the scientific method, accuracy and precision, drawing graphs and have a basic understanding of spectroscopy.
- Prepare bags with three–five different types of coins (with different weights), a total of nine–15, so enough for three trials each. Different-sized washers could be used as an alternative.

General equipment

- Ramp – door stops are ideal
- Two blocks – jenga pieces are ideal
- A hairdryer
- Metre ruler
- Coins
- Balance
- The **teacher's project guide** has a deflection graph – one needed per group (to be printed A3)

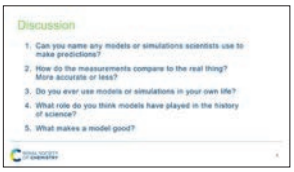
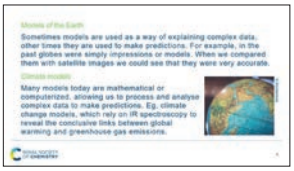
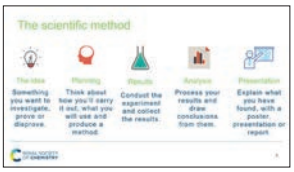
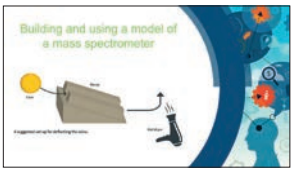
Additional resources

- For use with the suggested lesson plan PowerPoints, the **teacher's project guide**, the **class project instructions** and the **student project portfolio**.
- Visit **edu.rsc.org/resources/analysis** for information and resources for teaching about spectroscopy.
- Professional development course on scientific models and theories **rsc.org/cpd/resource/RES00001448/developing-and-using-models**

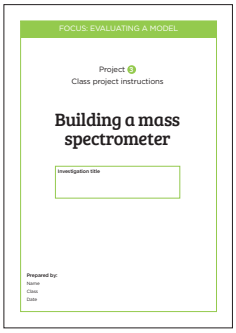
Model of mass spectrometer

This activity has been adapted from Rosie Research's *Making a Mass Spectrometer* **rosieresearch.com/making-mass-spectrometer**, which includes a video of the set-up.

BUILDING A MASS SPECTROMETER: LESSON ONE
Planning the project and carrying out the investigation

STAGE/PURPOSE	RUNNING NOTES	
Engage Get students interested in planning an investigation and how they would do it. Introduce them to some of the vocabulary.		Display slide 2 shows the question, what is the purpose of a scientific model?
		Slide 3 suggested answers: **1** Weather, climate change, particle models **2** It depends on the equipment usually and the input. **3** Video games, algorithms, weather forecasts **4** Notable ones include the solar system, the shape of the Earth **5** Robustness, reliability, track record of predictions
Real world and careers link Get students interested in how this links to their career aspirations and industry in Ireland.		Display slide 4 shows how this is relevant to the real world. An interesting article to challenge higher level students and those who want to know more about the modelling: T R Anderson, E Hawkins, P D Jones, *Endeavour*, **40**, 2016, 178. DOI: 10.1016/j.endeavour.2016.07.002.
		Display slide 5 shows a condensed personalised version of two careers stories.
Scientific method This section allows teachers to introduce key concepts for undertaking the scientific method.		Display slide 6 shows the key stages of the scientific method which students should be aware of throughout their projects, relating what they are doing to each of the key concepts.
Project instructions and investigation Students should be encouraged to play around with the equipment before deciding on a method and collecting results.		Display slide 7 **1** Put students in groups and give each group a copy of the **class project instruction** sheets. **2** Then give each student an individual blank **student project portfolio**. **3** Allow them then to plan and investigate which method they will choose.

3

STAGE/PURPOSE	RUNNING NOTES
Building a model This stage will allow students to explore a scientific model and also engage with the knowledge in the curriculum (how a mass spectrometer operates).	It's ideal to provide the graph paper at the start of this session, after the students have experimented with a number of different methods. → The **class project instructions** contain comprehensive help with how to collect results and conduct the analysis. 
Probe The students gain first-hand understanding of how models generate results.	Students should be guided to understand that the model seeks to prove or demonstrate how coins can be separated by their variability in mass, and that deviation from these results points to a lack of robustness in methodology. This hopefully infers an understanding that models, and the results they generate, are subject to the rigorousness of the planning.
Analysis conclusion	This section allows teachers to draw attention to the difference in the model and the key concepts for undertaking of the scientific method.
Evaluation of the model Including learning the differences by focusing on what a mass spectrometer actually measures.	This involves answering some applied questions which will extend their understanding of the mass spectrometer and thus will extend their ability to evaluate.
Extension task	An extension task for this section is included in the research section at the end of the **class project instructions**. It is not part of the project as it is not required for the Leaving Certificate specification but could challenge higher lever students.

Project 3

Teacher's project guide

Building a mass spectrometer

Building and using a model of a mass spectrometer

Why are you doing this investigation?

What do you want to find out?

We are investigating whether you can separate out coins based on their weight.

How?

Through the design of a method which exploits the differences in this variable (mass of the coin), by applying force which distinguishes them.

Why?

To explore the concept of a scientific model, while gaining an appreciation for the robustness of method to give accurate data.

3

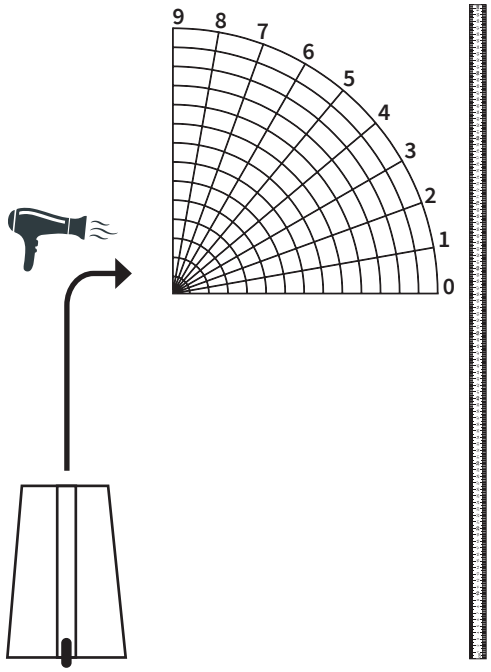
Suggested method

A suggested set-up is outlined here, and an A3 sheet of deflection angles is included. A metre ruler makes a good stopping point for the coins and provides an alternative metric for the distance travelled, and can be combined with the angle by the use of string.

However, it could be observed that more convoluted steps will confer a less robust method.

Students should be encouraged first to try and work out how to measure the deflections. Most distances and variations are acceptable, so they should be encouraged to find what generates the best results for accuracy and precision. For example, too close to the hairdryer causes the coins to be blown across the page rather than to roll.

Students could be made aware that each coin represents an isotope of the same element.



Variables

Students should be encouraged to identify their own variables and design for how they will obtain the most accurate results.

Make sure that students are aware that consistency with their execution of the method is required to get accurate results. This includes placing the hairdryer and the ramp in the same place each time, and also considering the force with which they release the coins each time.

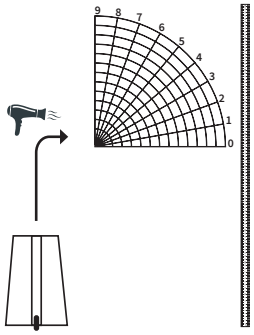
Independent – the mass of the coin

Dependent – the angle of deflection

Control – the power of the hairdryer, coin release force, height of ramp

Results

Raw data



Mass (g)	Average angle of deflection
2.3	90.0
	89.0
	89.0
3	91.0
	90.5
	88.0
3.6	70.0
	69.0
	71.0
7.1	69.0
	68.0
	66.0

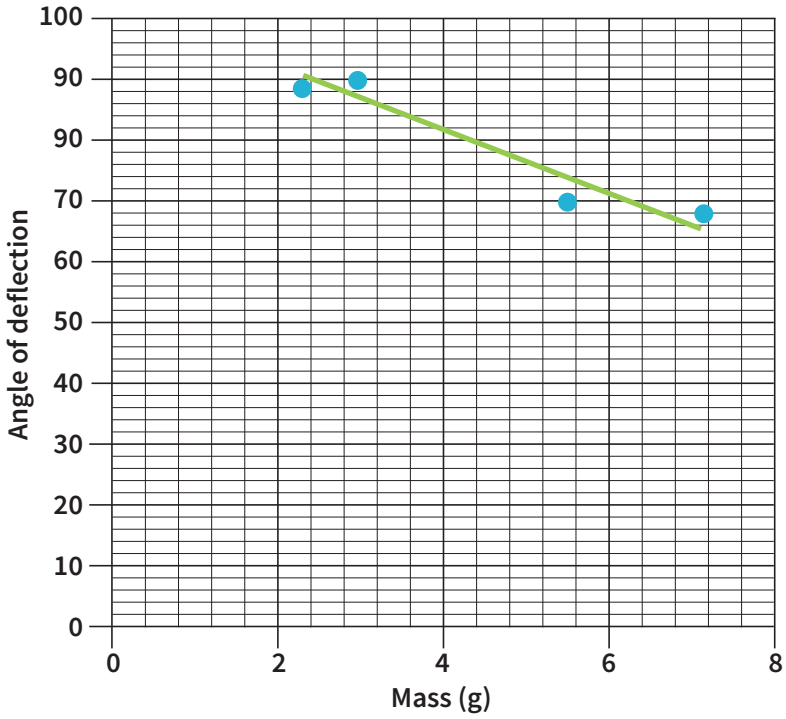
Results could be collected with the angle graph or using a metre ruler to gauge relative distances.

Averaged results table

Mass (g)	Average angle of deflection
2.3	89
3	90
5.5	70
7.1	68

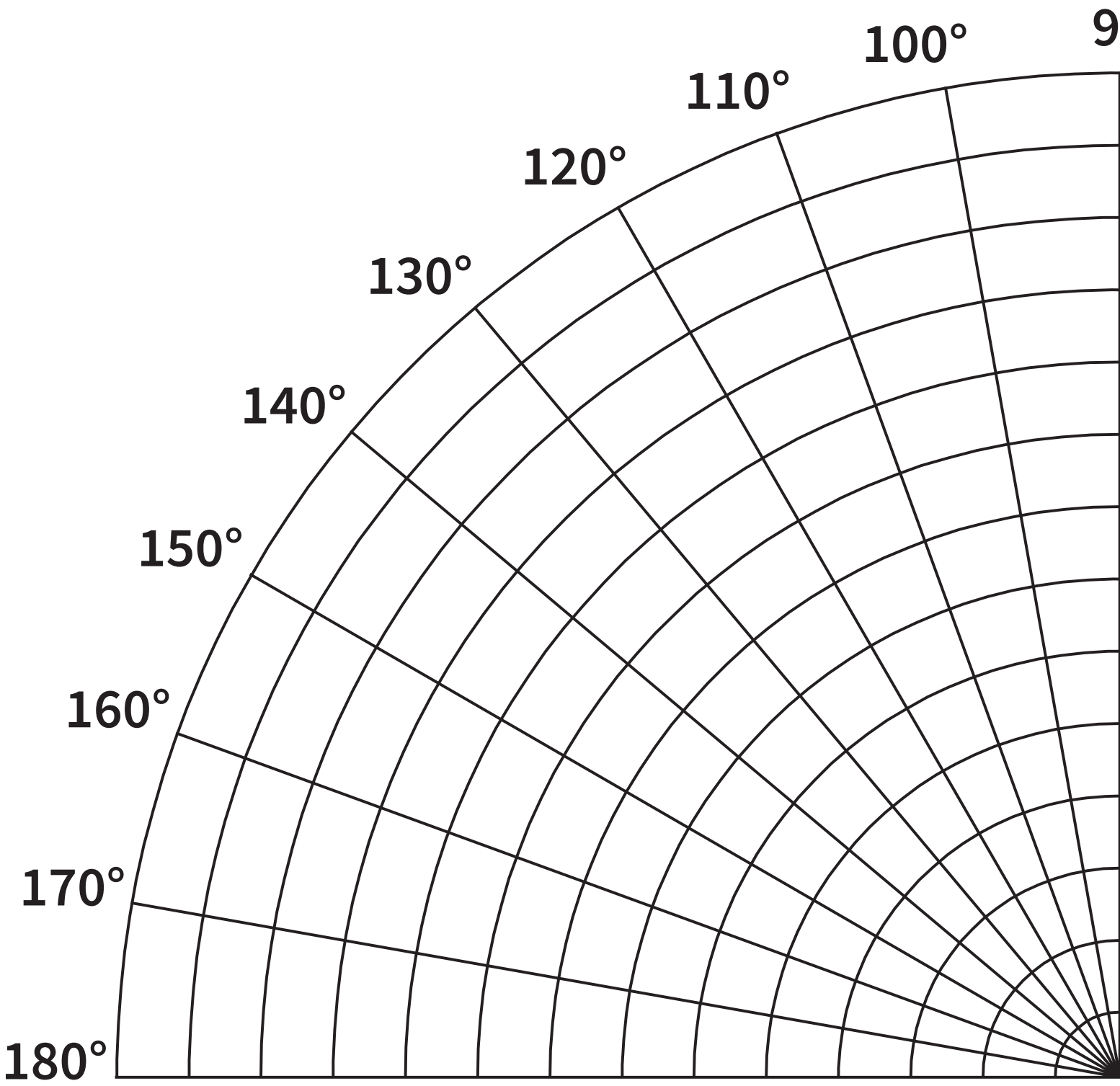
Graph

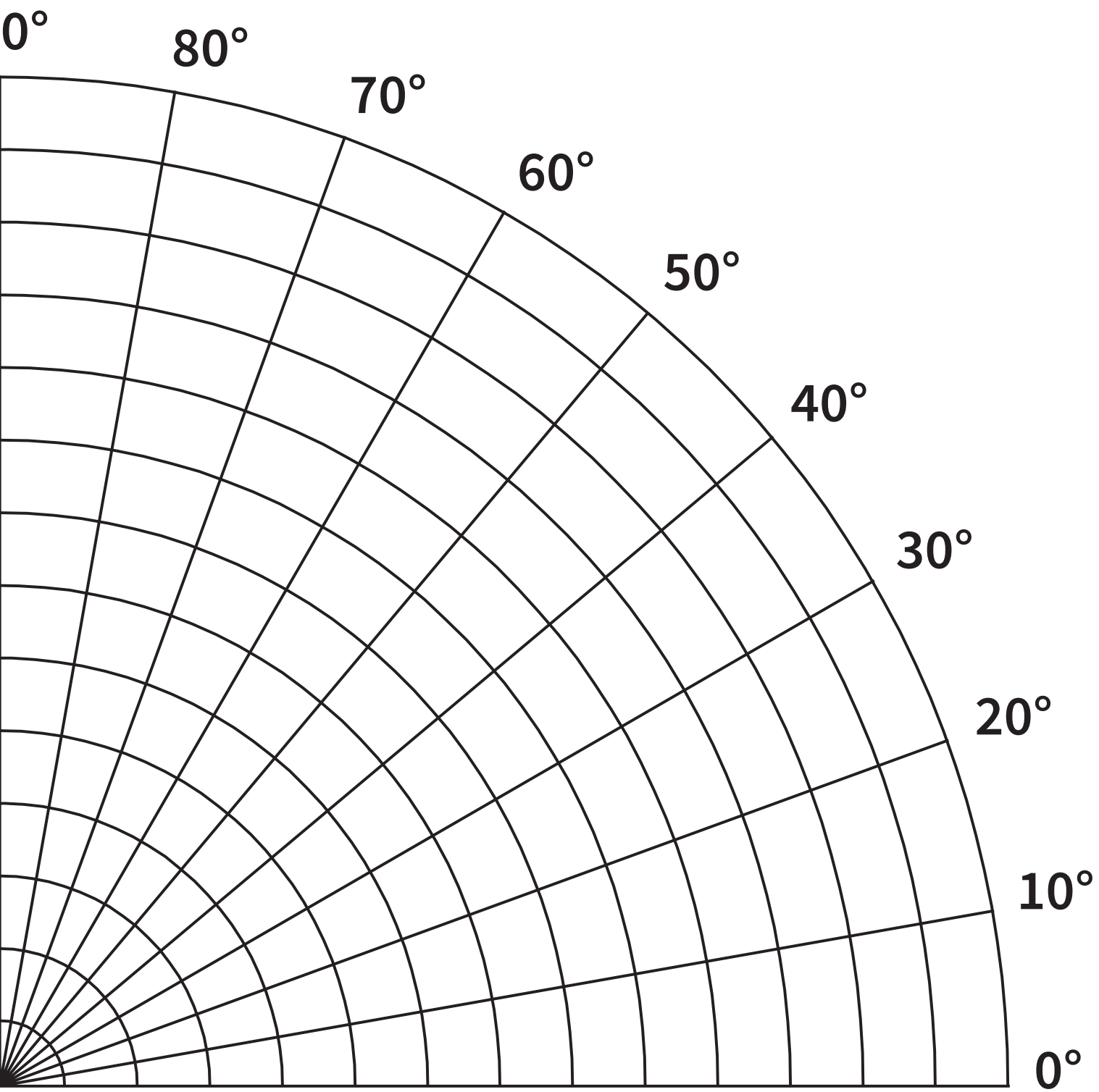
The following graph provides a representation of the results for four different coins, allowing for a more conclusive data set and hence a line of best fit to illuminate the general trend, ie that as the mass increases the angle of deflection decreases. This observation is not important for the knowledge of mass spec but serves to represent a key feature of how it works, by the deflection column.



Students should be encouraged to peer mark their graphs using the sheet in their group guide.

Deflection graph template




0°
80°
70°
60°
50°
40°
30°
20°
10°
0°

3

Graph analysis

Describe the relationship that has been established between the independent and dependent variables and link this back to the theory if possible.

Checklist for analysing the graph

1 Make a statement describing what the graph shows, or the relationship between the two variables, eg 'As the mass increases, the angle of deflection decreases.'

2 Use the results, usually two as evidence, eg 'When the mass was 2.3 the deflection was 89 degrees. When the mass was twice this size the angle of deflection was …'

HL 3 Link this to the model explaining what this model represents, eg 'These results would reflect what is to be expected, a larger mass leads to a higher degree of deflection therefore …'

Conclusion

How could you improve your results next time?

For example, what would you change about your method, or the day/location/the amount of time taken to get accurate results? Hint! Think about the following:

- uniform circumference of the coins
- a way to remove wind resistance

Or interestingly, what would happen if you had a greater discrepancies between the sizes of the coins?

Here we want to point out the parallels between the difficulties in obtaining significantly different deflection results and the problems scientists face with minute particles in the real-world. This is why advanced mass spectrometry techniques that measure the mass coupled with the charge (m/z ratio) are significant, they have increased sensitivity as they allow for a wider variability in the results.

Make a concluding statement linking back to your hypothesis, suggesting whether your results confirmed or denied that, eg 'My results confirm that as the mass increased the angle of deflection increased, this works the same way as in a mass spectrometer suggesting that the model was relevant or accurate as a demonstration.'

How does the model of a mass spectrometer compare to an actual instrument?

- It accelerates coins using a force (in a mass spectrometer this is an electric field, in the DIY spectrometer, there is ramp to introduce the force of gravity).
- It uses a secondary force to change the path of the sample (in a mass spectrometer this is a magnetic field where deflection changes based on the mass and charge of the ions, in the model mass spectrometer, this is a force of the hairdryer that changes based on cross-section and mass of the coin).
- It separates objects based on mass (in a mass spectrometer this can be isotopes in a carbon sample like ^{12}C and ^{14}C and in the DIY mass spectrometer this is the type of coin).

Project 3

Class project instructions

Building a mass spectrometer

Investigation title

Prepared by:

Name

Class

Date

Building and using a model of a mass spectrometer

Background

Mass spectrometry (MS) is a very useful analytical technique that takes advantage of the mass to charge ratio (m/z) in a sample to determine its identity. The technique is about 1000 times more sensitive than infrared or nuclear magnetic resonance analysis. Extremely small samples (a few nanograms) can be analysed using MS.

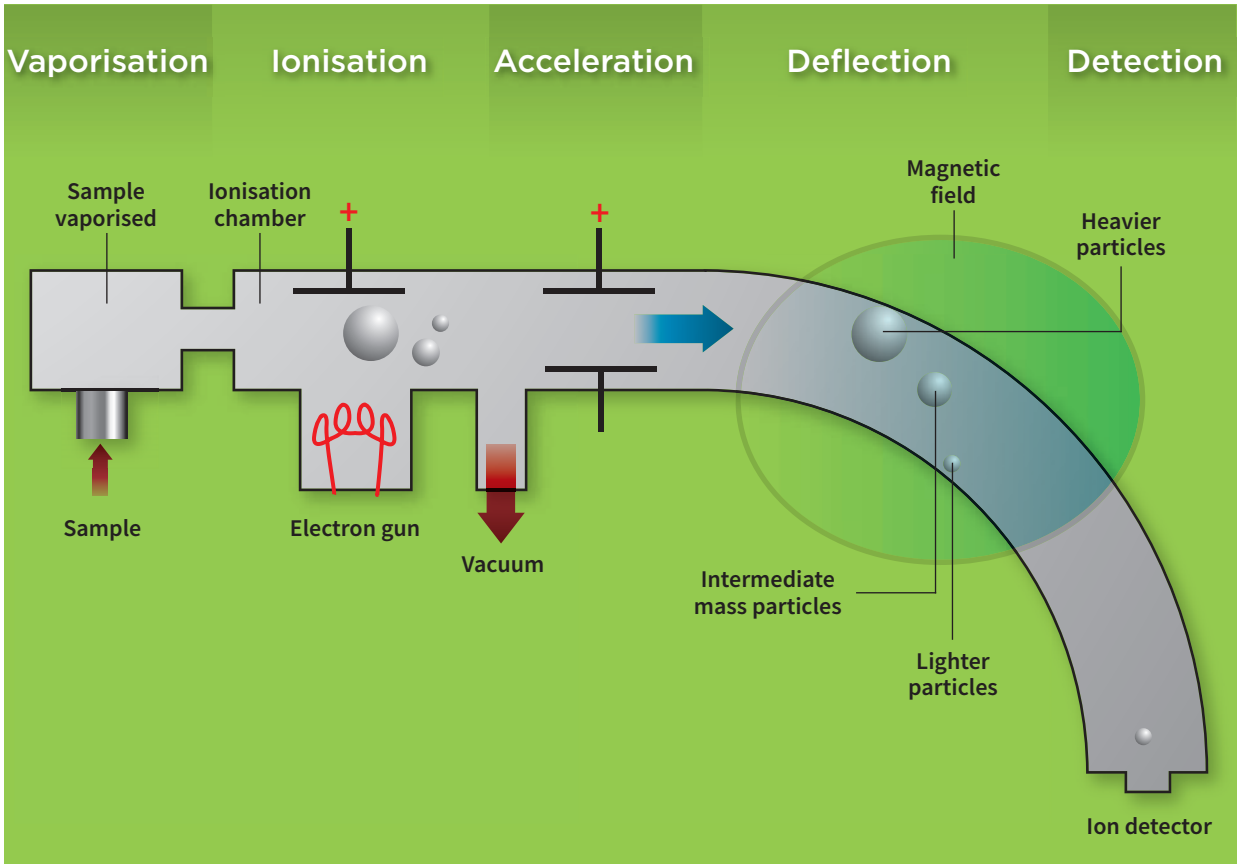


Diagram depicting the main principles of MS

It takes the particles through the process outlined below. For more details, including an interactive simulation, follow the link **edu.rsc.org/resources/mass-spectrometry-ms/11332.article**

How it works

MS uses quite sophisticated equipment and techniques to separate samples. First they are **vaporised** and then **ionised**, which will give them a charge. Then they are **accelerated** down the chamber, which contains a magnetic field designed to influence the charge on the particles. The chamber is also quite long and curved to allow the samples to be **separated** by their mass and ability to be deflected.

Your task

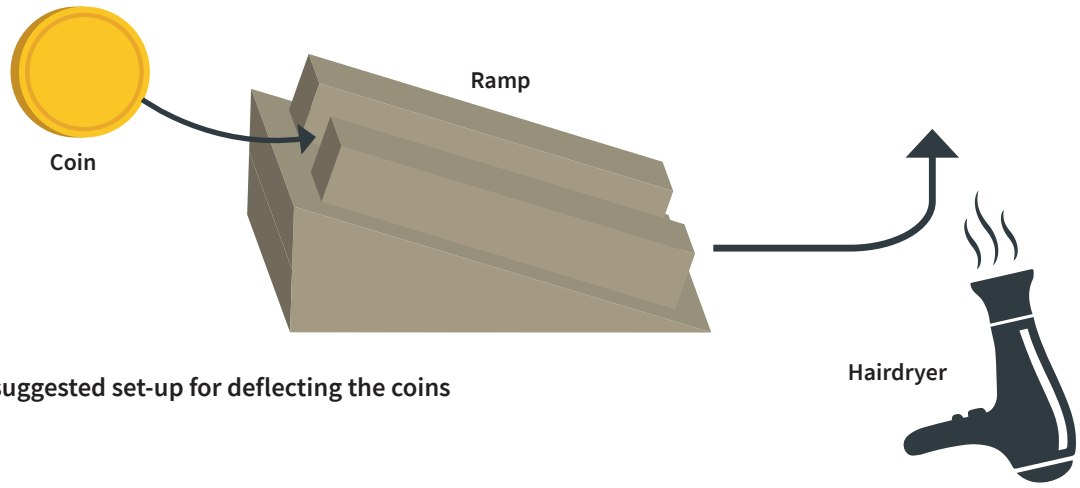
Your task is to create a model mass spectrometer, the best that you can! What will make it the best is how well it separates the bag of coins your teacher will give you.

You should design it to separate them by mass, using the same techniques as a mass spectrometer, ie some way of deflecting them and then measuring this deflection. The recommended set-up is outlined below, but you should be as creative as possible in your method.

Keep in mind that the best scientific methods are often the most robust, ie are resistant to errors, and can be completed a number of times and still generate the same results.

Your teacher will give you a bag containing at least two different types of coins.

Construct your own set-up as shown below.



A suggested set-up for deflecting the coins

Consider how your model of a mass spectrometer compares to an actual instrument.

- It accelerates the sample using a force (acceleration)
- It uses a secondary force to change the path of the sample (deflection)
- It separates objects based on mass (separation)

Think about how you could measure the deflection of the coins.

BUILDING A MASS SPECTROMETER
Planning sheet

Why are you doing this investigation?

What do you want to find out? This could be some type of hypothesis or idea you want to prove or disprove, or a way to explain a complex process.

Include any inspiration for undertaking the project, eg the work of other scientists (particularly anything from the careers stories), or things in the media that might have motivated your interest in this topic.

What do you think you might discover or find? This should link to the focus of research and analysis, and how your results will prove or disprove your hypothesis or idea.

Deciding your method

Your equipment should give you an idea of how to set up your method – try to focus on achieving the most repeatable results.

Variables

What are your project variables, including control variables?

Are there any control variables that you will not be able to control, and what impact do you think this will have on your results?

Model

For the focus of the evaluation, you should seek to make your model represent a key feature of how the mass spectrometer works, aiming for a model that does one thing well rather than many things less accurately.

3

Include a photograph or a diagram of your equipment set-up

Results

Models are particularly well suited to qualitative evaluations, eg how it was both like and unlike the real simulation.

Raw data

This should be a table of results you collected, without any processing. Careful! This model seeks to demonstrate something we already know to be true, and when collecting results, you should discard those trials where there was clearly a physical cause, such as the coin wobbled, or it went over a bump in the floor. If there are consistencies with this, it points to your method needing to be changed, eg the coin with a dent in it continually veered left, so this coin should be removed from the sample.

Averaged results table

You should average your trials – usually you will have about three. This means add them all together and divide by three (if you carried out three trials).

For quantitative data, analysis involves collecting numerical values, using this to carry out calculations or presenting the numerical values in a graph to establish a relationship between independent and dependent variables or to find an unknown value.

Graph

Graphs should only be drawn from averaged results.

Draw your graph by hand or on Excel and paste it in the box below.

Affix graph here

Marking criteria for the graph

- Axis drawn using a pencil and a ruler.
- Axis labelled with correct headings and includes units.
- Appropriate scale used.
- Points plotted correctly.
- Line of best fit drawn.

Describe the relationship that has been established between the independent and dependent variables and link this back to the theory if possible.

Checklist for analysing the graph

1 **Make a statement describing what the graph shows or the relationship between the two variables**, eg 'As × increases, y decreases because …'

2 **Use the results, usually two as evidence**, eg 'When the mass of the coin was two grams, the coin was deflected by × degrees. When the mass of the coin was four grams, the coin was deflected by 2x degrees'.

HL 3 Link this to the theory explaining why this relationship exists, state whether the hypothesis or question posed at the beginning of the investigation is correct, eg 'These results would reflect what is to be expected, a greater mass corresponds to a higher degree of deflection, therefore …'

Conclusion and evaluation

How could you improve your results next time? For example what would you change about your method to get more accurate results?

Make a concluding statement linking back to your hypothesis, suggesting if your results confirmed or denied that. Also include what you have learned from the project and any suggestions you may have for proving or disproving the method.

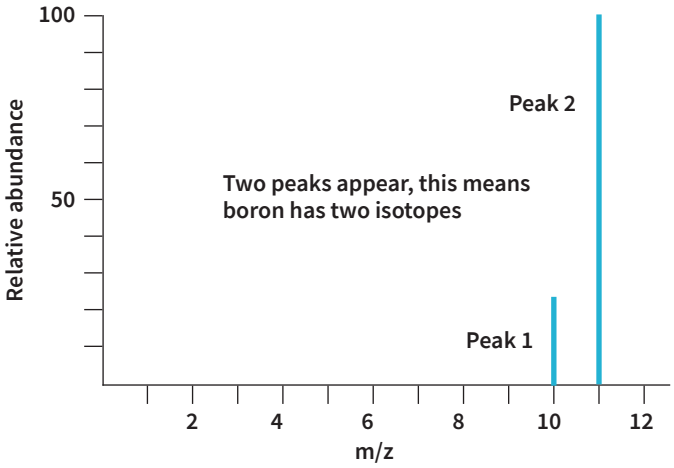
List the key ways your model differs from a real mass spectrometer. Why was a ramp used, what is this analogous to in an actual mass spectrometer? What did the hair dryer represent? Why were different sized coins used?

BUILDING A MASS SPECTROMETER
Research

Mass spectrometers in industry are used in a variety of ways and with a number of different techniques. In the careers stories section, you will see that they are often used to identify substances.

Luckily, you don't have to interpret these graphs but you have to be familiar with how some of the simpler ones work, such as how the relative atomic mass of an element is calculated from the relative abundance of its isotopes.

All that means is imagining back to your bag of coins – an element can exist in a number of different forms called isotopes (or coins). If you know the number of different coins and the total mass of them then you could calculate an average for a single coin that is the relative atomic mass or Ar, which is what the following graph represents.



Graph shows the mass spectrum produced for a sample of boron. See chemguide.co.uk/analysis/masspec/elements.html

Calculation

To calculate the relative atomic mass of boron (as shown on the periodic table):

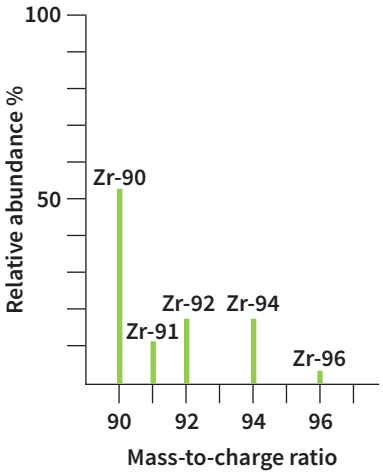
STEP ONE Take the mass to charge ratio (m/z) and multiply it by the relative abundance of the isotope. Calculate this for all isotopes detected and add together.

1 [11 (m/z) × 100 (relative abundance of isotope 1)] + [10 (m/z) × 23 (relative abundance of isotope 2) = 1330.

STEP TWO Then divide this by the total relative abundance to get the weighted average for one boron atom.

2 1330/123 (combined relative abundance of isotope 1 and 2) = 10.8

The peaks in the graph show the relative abundance of the two most common naturally occurring isotopes of boron and its Ar reflects their distribution between 10 and 11.



Graph shows mass spectrum of zirconium

Challenge

The relative abundance of zirconium is shown on the left. Using this graph, calculate the relative atomic mass using % abundance.

Hint! It works the same way as mass but using percentage instead.

Project 3

Student project portfolio

Building a mass spectrometer

Project title

Prepared by:

Name

Class

Date

BUILDING A MASS SPECTROMETER
Planning sheet

Why are you doing this investigation?

Deciding your method

Variables

Model

Include a photograph or a diagram of your equipment set-up

3

Results

Raw data

Averaged results table

Graph

Affix graph here

Marking criteria for the graph

- Axis drawn using a pencil and a ruler.
- Axis labelled with correct headings and includes units.
- An appropriate scale was used.
- Points plotted correctly.
- Line of best fit drawn.

Analysis

Conclusion and evaluation

Your answer for the challenge question

Project 4

Research and analysis

The sunshine factor

- Themed lesson guide for teachers
- Teacher's project guide
- Class project instructions
- Student project portfolio

THEMED LESSON GUIDE FOR TEACHERS

The sunshine factor

Focus: **research and analysis.** Two lesson plan

4

Task

Investigating how sunscreens are effective.

Background

This investigation provides a summative task for the understanding and skills gained in the previous projects, observation and inference, accuracy and precision, graph skills and culminates in 'analysis', allowing the students to consolidate and demonstrate their knowledge so far. It can also be used as a standalone project to inform students about ultraviolet (UV) rays and how sunscreens are used to combat some of their detrimental effects.

Learning objectives

On completion of the project students will:

- relate UV rays, the sun and sunburn;
- recall what sun protection factor (SPF) is and describe how different sunscreens achieve this;
- plan and evaluate a a scientific investigation to test some of the features of sunscreen.

Pre-planning

- Ideally, students will have completed the previous projects to gain a solid understanding of the scientific method, accuracy and precision and drawing graphs, and have a basic understanding of spectroscopy.
- UV beads will need to be ordered in advance (at least eight per group of students).
- Best on a sunny day with little cloud cover.

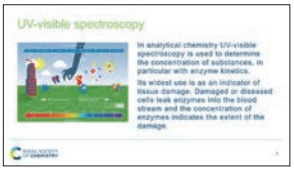
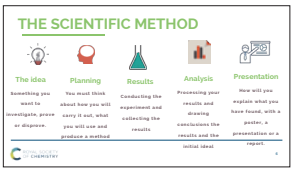
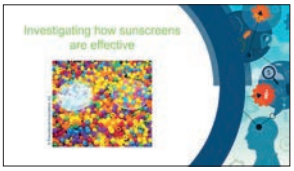
General equipment

- UV-sensitive beads
- A clear covering on which to apply the cream
- Suggestions: acetate/overhead projector sheets/microscope slides and lens covers. Plastic sandwich bags can also be used but it is much harder to evenly apply the cream to these.
- Three different SPF sunscreens
- Balance (optional)

Additional resources

- For use with the suggested lesson plan PowerPoints, the **teacher's project guide**, the **class project instructions** and the **student project portfolio**.
- Visit **edu.rsc.org/resources/outreach-sunscreen-and-uv-light/1212.article** for information and resources for teaching about spectroscopy.
- Ireland Science on Stage video comparing suncreams by UV absorption: **vimeo.com/91604126**
- Free resource from Stanford Solar Centre **solar-center.stanford.edu/activities/uv.html**
- Read more about the chemistry of UV-detecting beads at **teachersource.com**. You can also find the free activity used as inspiration for this project and resource from Educational Innovations **s3.amazonaws.com/cdn.teachersource.com/downloads/lesson_pdf/UV-AST.pdf**

THE SUNSHINE FACTOR: LESSON ONE
Planning the project and carrying out the investigation

STAGE/PURPOSE	RUNNING NOTES	
Engage Get students interested in planning an investigation and how they would do it.		Display slide 2 shows the question: How are sunscreens effective?
		Slide 3 opens up the discussion about how we could measure this.
Real world and careers link Get students interested in how this links to their career aspirations and industry in Ireland.		Display slides 4 and 5 show how this is relevant to the real and global world.
		
		Display slide 6 shows a condensed personalised version of two careers stories.
Scientific method This section allows teachers to introduce key concepts for undertaking the scientific method.		Display slide 7 shows the key stages of the scientific method. These overlap with key sections in the **class project instructions**.
Project instructions and investigation		Display slide 8 which gives the title of the investigation and some indication of the method. At this point the **class project instructions** should be given. The video link below provides some inspiration on the utility and creativity that these beads can invoke. **vimeo.com/36033383** During this section students should be able to explore the best method for their investigation. Finally, when the group is clear about their method, give each student an empty **student project portfolio**. Ask them to individually fill in the planning section of the report and collect their data.

4

STAGE/PURPOSE	RUNNING NOTES
Project analysis This stage will allow students to apply their knowledge of UV and skills in the scientific method to explain some of its features of sunscreen.	Drawing graph and completing results analysis → The **class project instructions** section contains a comprehensive guide to conducting this analysis. There are research questions at the end of the **class project instructions** to be completed in advance or after students have completed the project. The answers can be found in the supporting **teacher's project guide**. 

Project 4

Teacher's project guide

The sunshine factor

Investigating how sunscreens are effective

Why are you doing this investigation?

What do you want to find out?

Whether it is possible to 'qualify' the effectiveness of a variety of sunscreens. The measurements will not be numerical, they will be of a qualitative nature.

Students should be encouraged to evaluate the method in terms of the previous foci, such as accuracy and precision.

There are options to compare it with UV apps and online indexes such as the Met Office Ireland, for a particular time and place (as referenced in **student instruction sheet one**.)

4

Suggested method

1 Conduct this activity on a bright sunny day.

2 Using the acetate sheets draw on a table with space for two/three beads for each SPF, as shown right.

3 Place one drop of sunscreen on the first layer over each bead.

4 Repeat this for the sunscreens available.

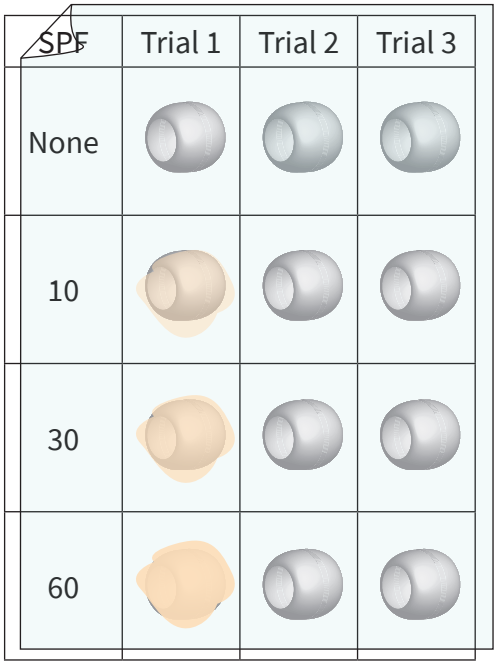
5 Then place another sheet over the top, gently pressing to give each bead an even coat.

6 Leave one row uncovered – this will act as a control so you can see the intensity of the colour change when no protection is offered.

7 Place the sheets in direct sunlight.

8 Wait 10 minutes to allow the detector beads to change colour. Record any colour change.

There are plenty of alternatives to this method, including simply spraying the beads an equal number of times, using plastic bags and trying to apply even coats, and microscope slides and covers.



Suggested set-up with acetate sheet over UV beads

Variables

Students should be encouraged to identify their own variables and design in how they will obtain the most accurate results.

Independent variable – the SPF of the sunscreen. Other variables could be the type or brand of sunscreen, although sufficient variation might not be measurable with such insensitive equipment.

Dependent variable – the intensity of colour on each bead.

Control variables – the amount of sunscreen will be difficult to control. Suggestions include one drop each or weighing the amount.

Other variables include the time in the sun and the colour of the surface behind the acetate sheets (where the beads sit, eg the ground, a white piece of paper) as greater reflection could influence the results.

Raw data

Trial 1	
Sunscreen SPF value	**UV bead detector colour intensity**
0 (no sunscreen)	
20	
30	
50	

Averaged results table

SPF	Colour intensity of bead	Intensity value
0	intense	4
20	medium intensity	3
40	light intensity	2
60	white	1

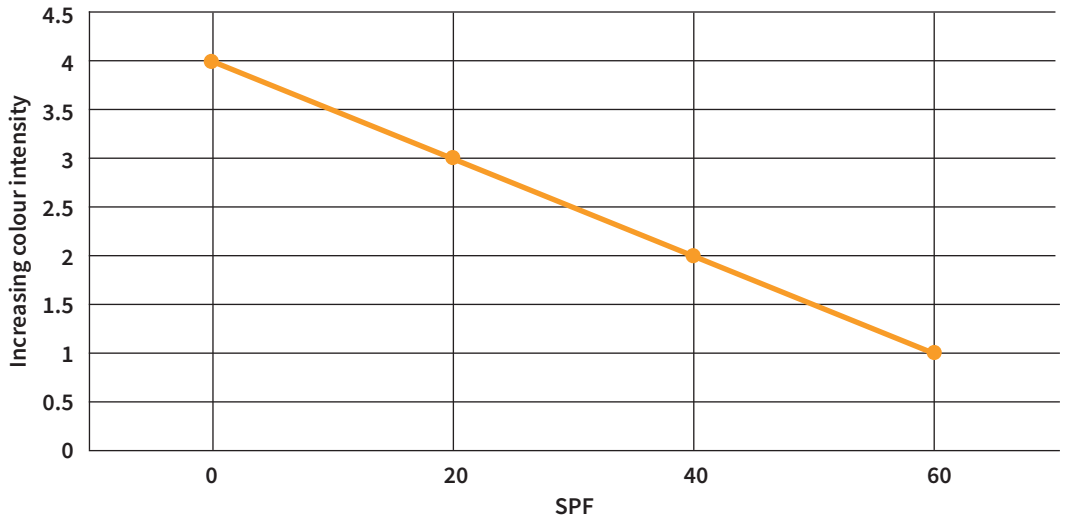
Graph

Students could be encouraged to draw a graph of the results, but often a table is sufficient for qualitative results, as the analysis remains the same.

Suggestions for transforming qualitative data include giving numbers to represent the intensity, eg white = 0 and intense = 4.

The advantages of this can be that it allows scientists to become less biased and often more precise (allowing for averages). It also allows patterns and trends to be realised more easily.

How the colour intensity of the UV bead changes with SPF



4

Graph analysis

Describe the relationship that has been established between the independent and dependent variables and if possible link this back to the theory.

Checklist for analysing the graph

1 Make a statement describing what the graph shows, or the relationship between the two variables, eg 'As SPF increases, the intensity of the colour of the beads …'

2 Use the results, usually two as evidence, eg 'When the concentration was 1 ppm the absorbance was 0.5, when the concentration of the standard solution was 5 ppm the absorbance was …'

HL 3 Link this to the theory explaining what this model represents, eg 'These results would reflect what is to be expected, a higher SPF means more sun protection, therefore …'

Hint! Reference could also be made to the wavelength of the most intense light and which colour this corresponds to on the UV-Index (shown in **student instruction sheet one**.)

Conclusion

How could you improve your results next time? What would you change about your method, or the day/location/time to have obtained more accurate results, eg more accurate application of sunscreen?

Variables that affect the strength of the rays reaching the ground:

1 time of day – UV rays are strongest between 10.00 am and 4.00 pm;

2 season of the year – UV rays are stronger during spring and summer months;

3 altitude – more UV rays reach the ground at higher elevations;

4 clouds – the effect of clouds can vary, but what's important to know is that UV rays can get through to the ground, even on a cloudy day;

5 reflection off surfaces – UV rays can bounce off surfaces like water, sand, snow, pavements or even grass, leading to an increase in UV exposure;

6 contents of the air – ozone in the upper atmosphere, for example, filters out some UV radiation.

Make a concluding statement linking back to your hypothesis, suggesting whether your results confirmed or denied it, eg 'My results confirm that as SPF increases the intensity of the bead colour decreased.'

THE SUNSHINE FACTOR
Answers to research questions

1. Ultraviolet A (UVA) has a longer wavelength, and is associated with skin aging. Ultraviolet B (UVB) has a shorter wavelength and is associated with skin burning.
2. High intensities of UV can lead to persistent damage to cells and even burning, which can lead to skin damage and even blindness.
3. Broad-spectrum sunscreens are the best, meaning those that protect against both UVA and UVB. An SPF of 15 is usually the minimum, but SPF 30 is recommended.
4. The SPF number gives an indication of how long you have before the UVB rays cause reddening of the skin, eg SPF 30 means it will take 30 times longer for the reddening to occur than if you did not have any protection.
5. The SPF tells you how much it protects against UVB but not UVA.
6. Sunblock usually contains ingredients that physically block and scatter the rays before they penetrate your skin, such as the minerals titanium dioxide and zinc oxide. Sunscreens usually contain ingredients (like avobenzone and octisalate) that absorb UV rays before they can damage your skin.
7. Water, insect repellent and also rubbing in the sunscreen can all lead to reductions in its protective effects.
8. The greater the concentration the greater the ability to block or absorb the UV rays.
9. Too little sunscreen will mean it cannot protect to that SPF level – if more is applied it will improve the protection but only up to that level (and not higher). In addition most manufacturers suggest reapplying every two hours.

Project 4

Class project instructions

The sunshine factor

Investigation title

Prepared by:

Name

Class

Date

STUDENT INSTRUCTION SHEET ONE
Investigating how suncreens are effective

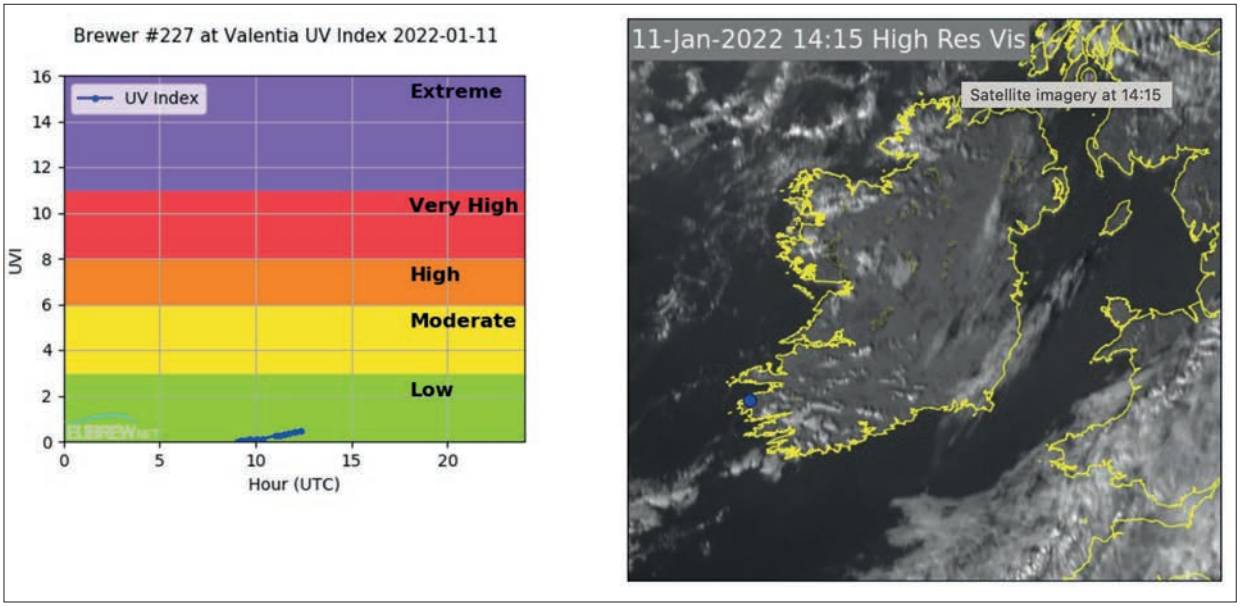
Background

The Earth's atmosphere prevents most ultraviolet (UV) radiation given off by the sun from reaching the ground. The radiation tends to be screened out by stratospheric ozone, which is about 35 km above the Earth's surface. UV radiation has both positive and negative effects.

Positive effects of UV radiation include warmth, light, photosynthesis in plants, and vitamin D synthesis in the human body. However, too much exposure to UV damages skin cells and can lead to wrinkled and patchy skin, cataracts and even skin cancer.

Sunscreens in the shops are labelled with an SPF (sunshine protection factor) number. This number tells you how good the cream is at absorbing UV radiation. The higher the SPF number the more absorption that takes place. Sunscreen contains molecules that can absorb UV radiation; this stops your skin absorbing the radiation and protects you from damage.

The Irish Meteorological Service (**met.ie)** and global weather stations often use the UV index when conveying information and advice on UV exposure to the public. It's the coloured index on the left-hand side. Unsurprisingly, on a cloudy evening in February the advice is that it's low. This might be something to think about in your investigation.



The UV index for Ireland on 11 January 2022

Your task

How it works

UV beads change colour when exposed to UV radiation. The greater the intensity of the colour the greater the exposure to UV light.

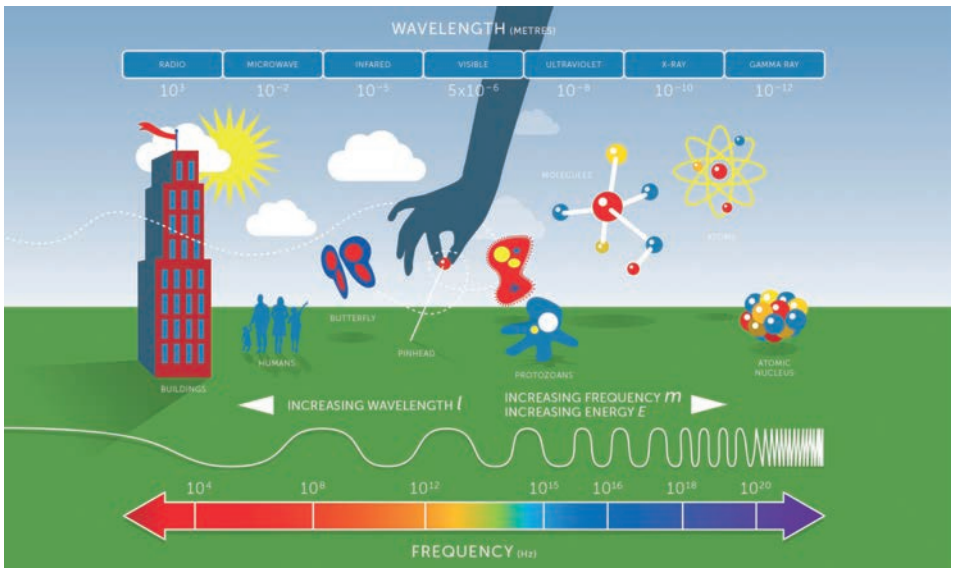
Your task is to test sunscreens to determine whether the higher the SPF number, the more UV light is being absorbed or reflected, offering better protection.

The electromagnetic radiation needed to cause a change in the colour of the beads is between 360 and 300 nm in wavelength. This includes the high-energy part of UV type A (320–400 nm) and the low-energy part of UV type B (280–320 nm).

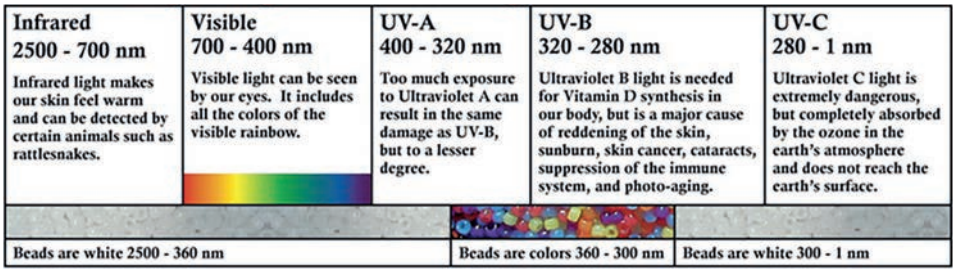
UV beads

Available from Educational Innovations, who offer a free activity resource for the beads at **cdn.teachersource.com/downloads/lesson_pdf/UV-AST.pdf**

The electro-magnetic spectrum and its corresponding wavelengths



Educational Innovations have provided this spectrum for their beads



You should design a method given the following equipment:

- UV-sensitive beads;
- a clear covering (eg acetate sheets) on which to apply the sunscreen;
- three different SPF sunscreens.

You could use: white, light intensity, medium intensity or intense when recording the UV bead colour intensity.

Planning sheet

Why are you doing this investigation?

What do you want to find out? This could be some type of hypothesis or idea you want to prove or disprove.

Include any inspiration for undertaking the project. The work of other scientists, weather warnings and sunscreen advertisements.

What do you think you might discover or find. This should link to the focus of research and analysis. How your results will prove or disprove your hypothesis or idea.

Deciding your method

Your equipment should give you an idea of how to set up your method – try to focus on achieving the most accurate results.

Variables

What are your project variables including control variables?

Are there any control variables that you will not be able to control, and what impact do you think this will have on your results?

Model

For the focus of 'research and analysis' you must include a hypothesis – this should be something you seek to prove or disprove, eg 'Paying more money means I get a better product'. You would then seek to prove or disprove this statement with your results.

4

Include a photograph or a diagram of your equipment set-up

Results

For qualitative data, analysis of the data can usually be done from the table of results as this requires making observations and the inferences from the observations.

Raw data

Averages are used by scientists to get a more accurate result. It allows for random variation and human error to be absorbed into the total, so increasing the accuracy.

This should be a table of results you collected, without any processing.

Averaged results table

You should average your trials – usually you will have about three.

This means add them all together and divide by three (if you carried out three trials).

For quantitative data, analysis involves collecting numerical values, using these to perform calculations or presenting the numerical values in a graph to establish a relationship between independent and dependent variables or to find an unknown value.

Graph

Graphs should only be drawn from averaged results. You should draw a graph of intensity against SPF.

Draw your graph by hand or in Excel and paste it here.

Affix graph here

Marking criteria for the graph

- Axis drawn using a pencil and a ruler.
- Axis labelled with correct headings and includes units.
- An appropriate scale was used.
- Points plotted correctly.
- Line of best fit drawn.

Describe the relationship that has been established between the independent and dependent variables and if possible link this back to the theory.

Checklist for analysing the graph

1 Make a statement describing what the graph shows, or the relationship between the two variables, eg 'As SPF increases, the intensity of the colour of the beads …'

2 Use the results, usually two as evidence, eg 'When the concentration was 1 ppm the absorbance was 0.5, when the concentration of the standard solution was 5 ppm the absorbance was …'

HL 3 Link this to the theory explaining why this relationship exists, state whether the hypothesis or question posed at the beginning of the investigation is correct, eg 'These results would reflect what is to be expected, a higher SPF means more sun protection, therefore …'

Conclusion and evaluation

How could you improve your results next time? What would you change about your method, or the day/location/time to have obtained more accurate results?

What system could you use to help you grade the effectiveness of each sunscreen?

Hint! edu.rsc.org/resources/mission-starlight/2073.article

There is a similar exercise in the Royal Society of Chemistry Mission: Starlight resource. You can use the graded colour chart shown here to consistently measure the colour change of each bead and compare it to a UV index.

Make a concluding statement linking back to your hypothesis, suggesting whether your results confirmed or denied that. Also include what you have learned from the project and any suggestions you may have for improving the method used to verify your hypothesis.

THE SUNSHINE FACTOR
Research questions

1. What is the difference between ultraviolet A (UVA) and ultraviolet B (UVB) radiation?
2. Why is prolonged exposure to UV radiation (light) harmful to the eyes and skin?
3. What protection from UV radiation should an effective sunscreen offer?
4. What does a sunscreen's SPF rating mean?
5. Does SPF tell us how well a product blocks UVA or UVB?
6. What is the difference between suncreens and sunblock (chemically)?
7. What reduces the effectiveness of sunscreen?
8. How will the concentration of molecules used in your final product affect how the sunscreen works?
9. How will the amount of sunscreen applied affect how it works?

Futher research links

1 **edu.rsc.org/resources/spectroscopy-in-a-suitcase-students-resource-spectroscopy-introduction/281.article**

2 D Dondi, A Albini and N Serpone, *Photochem. Photobiol. Sci*., 2006, **5**, 835. Available online **pubs.rsc.org/en/content/articlehtml/2006/pp/b606768a**

3 M Lucas, R E Neale, S Madronich and R L McKenzie, *Photochem. Photobiol. Sci*., 2018, **17**, 1956. Available online: **pubs.rsc.org/en/content/articlehtml/2018/pp/c7pp00374a**

Project 4

Student project portfolio

The sunshine factor

Project title

Prepared by:

Name

Class

Date

THE SUNSHINE FACTOR
Planning sheet

Why are you doing this investigation?

Deciding your method

Variables

Model

Include a photograph or a diagram of your equipment set-up

Results

Raw data

Averaged results table

Graph

Affix graph here

Marking criteria for the graph

- Axis drawn using a pencil and a ruler.
- Axis labelled with correct headings and includes units.
- Appropriate scale used.
- Points plotted correctly.
- Line of best fit drawn.

Analysis

Conclusion

4

Research questions

Careers and industry stories

- Introduction and curriculum links
- Careers and industry stories

Introduction and project links

This section contains career and industry snapshots of Royal Society of Chemistry members, particularly how their work involves analytical chemistry and instrumentation.

Analytical chemistry is the science of determining what elements or compounds are present in a given sample, separating it out, and measuring how much of it there is. All over the country this requires trained scientists and usually some very specialist equipment.

It is a key discipline in the world of chemistry; as the influence of technology increases, healthcare becomes more specialised and the need for sustainable solutions more pertinent. Many look to analytical chemistry to provide the answers and solutions, while for others, it begins with simply asking the right questions.

Industry and businesses in Ireland have responded to the needs and employ some of Ireland's highly skilled chemists. In this section they share how they use instrumentation and analytical chemistry in their work and careers. You can use these stories and applied examples to contextualise the work in this booklet.

Career and industry stories that link to one of the four projects are denoted by the project number. For example 1 links to Project 1 Emission Competition.

You can find more inspiring career stories and videos on A Future in Chemistry **edu.rsc.org/future-in-chemistry**

Scaling up 1

With the amount of plastic piling up in our oceans, the team at the radiation and environmental science centre at Technological University Dublin has been researching some green alternatives; turning shellfish waste into non-fossil-fuel-based plastics and coatings. Using spectroscopic techniques, the most effective extractions and treatments are optimised for scaled-up production. **Fionn Ó Fearghail**, lead researcher in the project, tells us more.

Ireland is geographically unique, and remarkable in that we have responsibility over an ocean area 10 times the size of our land. A vast natural resource which we utilise and rely on increasingly for products and services we use every day, from the fisheries to raw materials and even in the transport sectors.

At present, each year 70% of European shellfish biomass is ending up in landfills, incinerators or dumped at sea. Put to scale, that is 60 average sized, fully loaded container ships. Most of this waste material is the shells of the crustaceans. The shell is made up of three major components: a carbohydrate polymer, structural protein fibres and a mineral layer. There is a lot of interest in both chemical and enzymatic treatments of each shell component to extract and develop new materials.

There are already existing applications for the extracted materials in a range of industrial and consumer sectors including food supplements, fertilisers, coagulants and horticultural stimulants.

The carbohydrate polymer, known as chitin, is especially interesting because of its ability to form plastics, meaning we could potentially begin to move away from oil and fossil fuel-based plastics.

The most exciting thing about this idea is that the raw material is considered a waste product. This represents an attractive plastic alternative to use in the manufacture of household products as it is both cheaper and greener to produce.

Crab with a chitin shell

The major defining property of the extracted shellfish chitin is that it does not dissolve in any aqueous or organic solvents. This means that in order to determine the quality of this extracted chitin, to gain information on both its structural and molecular properties, we rely on the use of spectroscopic techniques. For use in bioplastics, the chitin must be treated either chemically or enzymatically to produce the soluble product chitosan.

After chitosan is dissolved in the necessary solvents, it can then be sprayed and cured to create thin films of durable and strong bioplastic – ideal for use in short shelf life or single-use products.

Spectroscopy in the form of ^{13}C nuclear magnetic resonance (NMR) allows us to compare quantitatively the insoluble chitin and soluble chitosan. Infrared and Raman spectroscopy are used to determine the purity and quality of the extracted chitin and chitosan. The spectroscopic analyses also allow us to compare how effective the extraction or treatment procedure was over another method. This allows for the extraction processes to be optimised; to be as cost effective, green and sustainable as possible when scaled up.

Thinking and discussion questions

1 What are the advantages and disadvantages of producing plastic from shellfish remains?

2 What implications could this research have for the Irish economy?

3 Why is it so important during the research stage to ensure your processes are as efficient as possible?

Carol Gleeson is a chemist in the human toxicology section of the State Laboratory, which provides forensic toxicology services to the Coroners Service of Ireland and the Office of the State Pathologist. Her skills are required to help these organisations to investigate the causes of an unexpected death.

When Carol's office receives a request, known as a toxicology analysis, she will conduct a variety of tests on the post-mortem samples. She will use a variety of spectroscopic techniques to test for the presence of prescribed drugs, illicit drugs and other toxic substances such as carbon monoxide. The quantity of the unknown substances is also determined. This is an example of qualitative and quantitative analysis. To produce these results they use high-resolution accurate mass spectrometry and then liquid chromatography mass spectrometry and ultraviolet (UV) spectrometry in the case of suspected carbon monoxide poisoning.

The silent killer

Every year carbon monoxide poisoning kills several people – it is called the silent killer because it's colourless, odourless, tasteless and non-irritating gas, which makes it very difficult to detect and even harder to determine as the cause of death.

Where does it come from?

When fuels are burnt, they often produce carbon dioxide and water, this is because the fuels are mostly made up of hydrocarbons (containing hydrogens and carbons) and heating this in air leads to the equation below.

Complete combustion

When we are able to burn all of the fuel, we call this complete combustion, but sometimes there aren't enough oxygen molecules available to react with the hydrocarbons, and the combustion is said to be incomplete. This causes different compounds to be produced – carbon monoxide and soot.

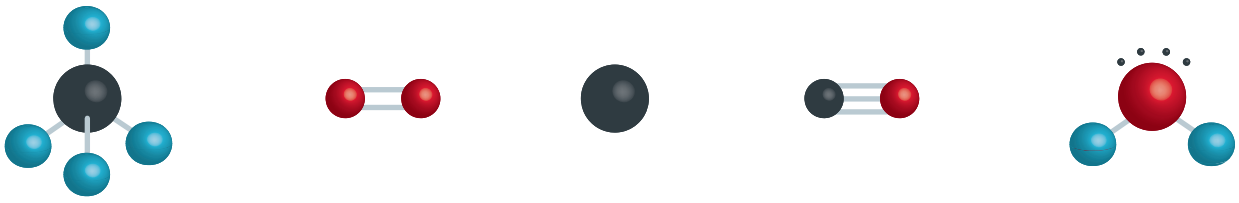
Incomplete combustion

Incomplete combustion is common in cigarette smoke and in vehicle exhaust fumes, where you can see the soot but not the colourless, odourless carbon monoxide.

Complete combustion: balanced equation

$CH_4\,(g) + 2O_2\,(g) \rightarrow CO_2\,(g) + 2H_2O\,(g)$

Incomplete combustion: balanced equation



$4CH_4\,(s) + 5O_2\,(g) \rightarrow 2C\,(s) + 2CO\,(g) + 8H_2O\,(g)$

Why is carbon monoxide a poison?

Haemoglobin is a red protein found in your blood and is responsible for carrying oxygen from the lungs to the different parts of the body. It binds to the oxygen molecules in order to carry and transport them. When it's in this carrying state it's known as oxyhaemoglobin, to show it's got oxygen bound to it.

However, picking up the right molecule is not always straightforward, in fact in the presence of carbon monoxide it will pick this up too. This forms the complex known as carboxyhaemoglobin (COHb) and the trouble with this is that once the CO molecules have bound to the haemoglobin it's very difficult to remove it.

Therefore, the haemoglobin is no longer free to transport the oxygen molecules. If this happens over a long period of time or there is a lot of carbon monoxide the result is often death from lack of oxygen.

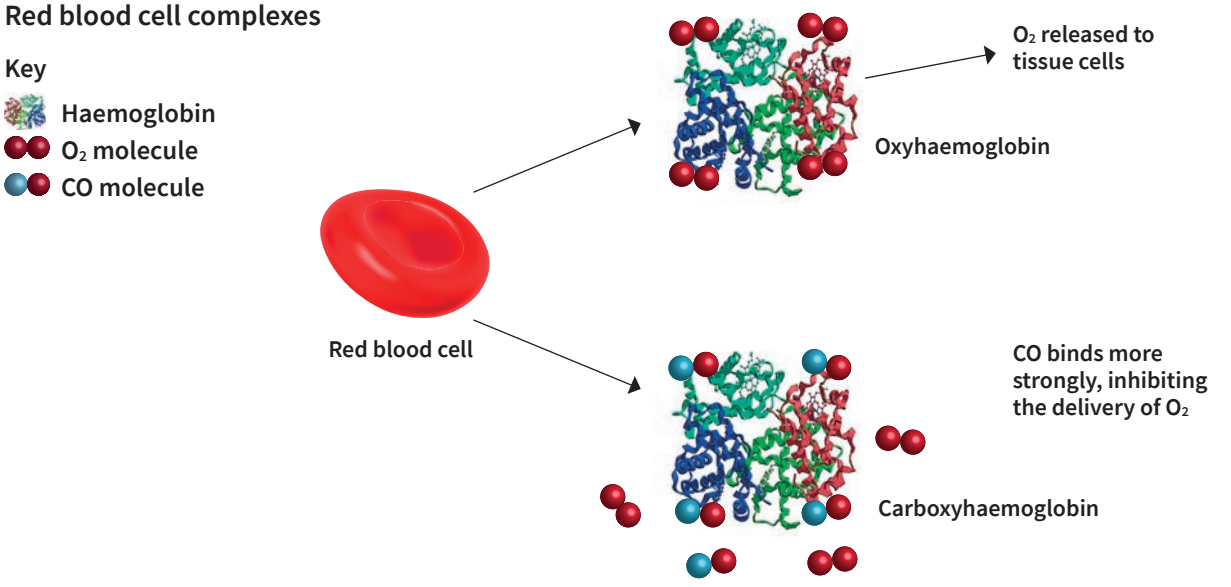
UV-visible spectroscopy is used to estimate the percentage of carboxyhaemoglobin present in the blood samples. The percentages of this give some indication of the cause of death, as shown by the results below.

- Carboxyhaemoglobin levels in the blood of urban non-smokers averages at 1–2%, and 5–6% in smokers.
- In 85 victims of fire, post-mortem carboxyhaemoglobin concentrations ranged from 25 to 85% with an average value of 59%. In victims of flash fires, however, carboxyhaemoglobin levels may not be significantly elevated.
- Analysis of a series of 41 fatalities due to the accidental or intentional inhalation of automobile exhaust gases has revealed carboxyhaemoglobin concentrations ranging from 48 to 93%, with an average of 72%.[1]

To run the UV-visible analysis Carol first must prepare her blood samples. She does this by diluting them with 0.01 M tris (hydroxymethyl) amino-methane and sodium dithionite solution.

To ensure quality control, blank samples demonstrate that the instrument is measuring accurately. External proficiency testing samples are analysed monthly and these results are assessed. The method validation is updated every two years. All samples are analysed in duplicate in two independent batches and an average result is reported.

Red blood cell complexes



Thinking and discussion questions

1 Why is chemical analysis so important in forensics?

2 What checks do Carol and her department carry out to ensure they are as accurate as possible with their conclusions?

3 Why is it important to have values on carboxyhaemoglobin blood concentration for smokers and non-smokers?

References
1 R C Baselt, *Disposition of Toxic Drugs and Chemicals in Man,* 11th Ed., 2017

HELPING FARMERS FEED THE WORLD
Quantitative and qualitative analysis

Cathal Connolly, associate director of research at Alltech explains how chemistry and chemists support food production.

What do you do in your day job?

I work a lot on fermentation and related processes, eg producing food and feed grade nutritional supplements, beverage alcohol (beers and spirits) along with management of co-product and waste streams. Also, I work on analytical method validation and verification for minerals of nutritional importance (eg selenium, copper and zinc, which are commonly used in health supplements) or finding out the levels of contaminants in process waste which may need to be reduced or removed so that they no longer present a threat to the environment, human or animal health.

My job is very varied and even though I have worked for the same company for several years, I have had the opportunity to work on many different projects in laboratories and production plants around the world.

I really enjoy working with a very diverse group of scientists and non-scientists in Alltech and with our many collaborations across the industry. We have close links with our education partners such as universities and other third-level institutions in Ireland and abroad. We are involved also at primary and secondary school level where we make presentations and demonstrations of how science works so that young children can gain a better understanding of why science is important and how it impacts their everyday life.

Tell us about how your work uses instrumentation

We are specialists in inductively coupled plasma mass spectrometry, a state-of-the-art analytical technique that is capable of detecting metals and several non-metals at concentrations as low as one part per quadrillion (ppq)!

We also use starch iodine titration both qualitatively and quantitatively. Qualitatively, we will use it in brewing scenarios, eg to test if all of the starch from the barley (malt) has been converted into fermentable sugars so that the yeast can metabolise it into alcohol (ethanol) and carbon dioxide during fermentation. This test involves a sample being taken from the tank and brought to the lab for a quick test 'by eye' following addition of a few drops of iodine (Lugol's solution). The formation of a black precipitate indicates the presence of starch so the enzymatic hydrolysis reactions might need more time for completion.

Quantitatively, we use titrations for measuring enzyme assay (ie we will check how active our enzyme has been at breaking down the starch). Initially, we will use the enzyme to hydrolyse (break down) the chemical bonds in our starch substrate (turning it into glucose) and then do a back titration using sodium thiosulfate to quantify the amount of starch that still remains.

Would you recommend a career in chemistry?

I'd really recommend to young people with an interest in a science career to consider the life sciences sector. An education as a chemist gives a superb grounding in analytical thinking that stands them in good stead for problem solving across the life sciences sector, from microbiology to biochemistry and biotechnology.

A degree is essential in a research line of work, because a certain depth of understanding of the subject matter and the scientific method is required when trying to figure what went wrong in an experiment or how to improve your results. It also helps when troubleshooting problems at the analytical end, including coming up with solutions to (ideally) solve problems before they happen.

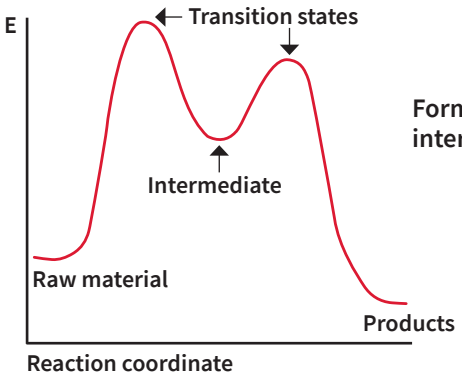
For some applied back titration questions relating to Cathal's work, go to page 139.

ENSURING DRUG QUALITY
Using infrared spectrometry

Ryan Sipho Twantwa, a quality control chemist at Pfizer, explains how he uses infrared spectroscopy to ensure the medicines they produce are correct, safe and effective for their patients.

I use Fourier transform infrared (FTIR) instrumentation and spectroscopy to test for and confirm the presence of functional groups in a specific sample.

Firstly, I seek to identify the substance using the IR spectra, this is known as qualitative data. Then to generate quantitative results I produce an absorbance concentration graph for the substance, which allows me to make the calculations necessary for my quantitative analysis.



A typical task involves testing the raw materials before they are used in the production process. This is to remove the potential for problems later on, especially when they become intermediates, a substance formed during a middle step of a chemical reaction between reactants and the desired product.

Further to this we also have to conduct a test to confirm that the steps are occurring correctly and will therefore yield the product we want. Finally, when we have a finished product it is then tested again to confirm whether the product reaches our standards.

Interestingly, the testing specifications differ based on which markets the drug is being sold to Africa, Europe, Asia or the US.

In a typical day, I would have to use the FTIR instrument and test a sample, but before I test anything:

1. I check the instrument is working properly and is functioning, ie that it is not damaged or due for maintenance;
2. I calibrate the instrument, and it must pass this test before I can use it. To calibrate the instrument I have to run a background check, which means a spectrum is taken of the experimental conditions to confirm the IR intensity without a sample;
3. I run through a reference sample, a pure compound that has the same components and functional groups;
4. finally, I run my sample and compare its spectra against that of the reference material – they should look identical.

If the IR spectra are not identical then the product cannot be used in the manufacturing process – I will inform the supervisor and further investigations will need to be carried out. Purity and consistency are fundamental to my job as these samples are going to patients all over the world and have to pass regulations and approval by authorities before they are sold. That is why great care is taken when working with samples, whether raw materials, intermediates or finished product. It is our legal and obligated responsibility as scientists to provide a correct, safe, quality and effective medications.

Thinking and discussion questions

1. Why might the drug specification change depending on which market it is being sold in and what are the implications of this?
2. Why is it so important to calibrate instruments before using them?
3. Why is quality control so important?

Aaron Power talks about working to improve a method for the detection of small quantities of heavy metals, while completing his master's placement with Environmental Laboratory Services in Cork.

I completed my master's thesis at University College Cork in 2014, where my research was based on measuring the amount of heavy metals in water samples.

Being able to complete an industry-based placement at Environmental Laboratory Services near Mahon was invaluable to this. The team there were trialling a new method which could more accurately measure the presence of heavy metals in pharmaceuticals.

The older method, which is known as the heavy metals test, has been used in the pharmaceutical industry for over 100 years. It is a colorimetric test that uses the chemical reaction of the heavy metal with a sulfide solution, and compares it with a standard prepared from a stock lead solution.

It is a limited method because it cannot tell you the concentration of metals in the samples, eg amount of lithium. Nor can it tell you the type of osmium present. One of the drawbacks of this method is that the colour change must be compared very quickly after the formation of the precipitate, and many analysts may read the results differently.

The improved method was to use a spectroscopic technique called inductively coupled plasma mass spectrometry (ICP-MS). The advantage of ICP-MS is that it can show exact quantities of each metal in the sample, including the presence of different isotopes.

Testing for heavy metals

The accuracy in this method is most important for metals such as arsenic or mercury. The metallic version of arsenic is the dangerous form while the methylated form can be found in seafood such as prawns.

With mercury it's a different story – in its methylated form it was the cause of the Minamata disaster. This was where a chemical factory in Japan sent methyl mercury out into the water table and as a result a lot of people and animals died from mercury poisoning.

Methyl mercury molecule

Thinking and discussion questions

1 Why was it important to test for the different isotopes of each metal?

2 Why are scientists always trying to improve the method they use?

3 Research the Minamata disaster and suggest how a more rigorous scientific method could have prevented it.

SOLVENT EXTRACTION AND MASS SPECTROSCOPY

Resolving a sticky situation 1

Edward Everson from Kerry Group gets a complaint from a customer who suggests her jam filling has a funny smell and taste. The team investigates, using solvent extraction and gas chromatography-mass spectrometry, to get to the bottom of the mystery.

The customer's sample is an orange filling which is usually made up of sugar, fruit, preservatives and flavour compounds. The team suspect it is the flavour that is to blame so they need to separate these compounds from the other ingredients. To do this they use solvent extraction.

1. The sample is first mixed with a solvent – typically dichloromethane or diethyl ether – in a separating funnel.
2. The mixture is shaken and then allowed to settle so that the phases separate out.
3. The solvent layer is then separated from the concentrate using a rotary evaporator.
4. This removes the bulk of the solvent, leaving behind a concentrated extract of the flavour components.

This extract would then be injected onto a gas chromatography-mass spectrometry instrument, which separates out the individual compounds so that the mass spectra can be used to identify each one. By running a standard sample as well as the complaint sample, it makes it a lot easier to identify what differences are present. We would focus on identifying these – in some cases extra peaks, sometimes missing peaks or sometimes just different ratios of peaks.

Once we have these identified we would then look for typical occurrences, things that are part of the flavour (orange), like oxidation of the products from prolonged aging or storage,

Orange jam

reaction products or something just really weird! In this case it was some furfuryl compounds – definitely hydroxymethylfurfural, maybe some furfural, 5-methylfurfural and also some para-vinyl guaiacol.

The furfuryl compounds are the burnt notes that come from cooking sugar. This made us go back to the production site where further investigation showed they had changed the type of tank used to make the jam. Originally it was a tank with a coil heater and stirring, but the new one was jacketed heating with less or no stirring – so the jam was overcooking around the outside of the tank!

For more information see **airborne.co.nz/hmf.shtml**

Thinking and discussion questions

1. Why is standardisation of products so important in industry?
2. Why is the consistency of the method so important in industry?
3. What was the purpose of the mass spectrometer in this investigation?

TRADITIONAL MEDICINES
Identifying chemical fingerprints

Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

Helen Sheridan, associate professor in the school of pharmacy and pharmaceutical sciences at Trinity College Dublin, talks about her career in research and using analytical chemistry to gain a greater understanding of traditional medicines.

My research group has successfully identified a lead molecule from a plant used in Taiwanese traditional medicine, a project which involved a programme of medicinal chemistry and multiple preclinical stages of development (including human clinical trials.) To support this project, I also co-founded a spin-off company, Trino Therapeutics, and secured funding of approximately €13 million (£11 million). The journey from discovery to human trials took over 20 years. During this time, I published 70 research papers and I currently hold seven published patents.

The driving force behind my work is to find new therapeutic treatments for unmet clinical needs by investigating meaningful uses for natural molecules to address some of the greatest challenges of global health.

Basil – more than just a condiment

The basil plant, *Ocimum basilicum*, has a beautiful fragrance. Many of you will know it and have eaten it on pizza and in pesto. There is another closely related species, *O. sanctum*, which looks similar but smells different. This means that the plants are chemically different, as chemicals are responsible for the smell. Both plant species generate a complex oil in the leaves that is called a volatile or essential oil.

The oil is a complex mixture of small chemicals with low boiling points. *O. sanctum* is commonly used in Ayurveda, which is a system of medicine with historical roots in the Indian subcontinent.

O. basilicum oil is also widely used, but its medicinal properties are not as well explored as those of *O. sanctum*. Both species have been reported to have potential health benefits, such as helping neurocognition, boosting immunity, having anti-inflammatory effects and impacting on cardiovascular disease.

The chemical composition of *Ocimum* oil (and other plant oils and chemical extracts) varies depending on the genetic stock the plants are grown from and environmental factors that affect the biological synthesis of chemicals in the plant, such as the nature of the soil, climate, etc.

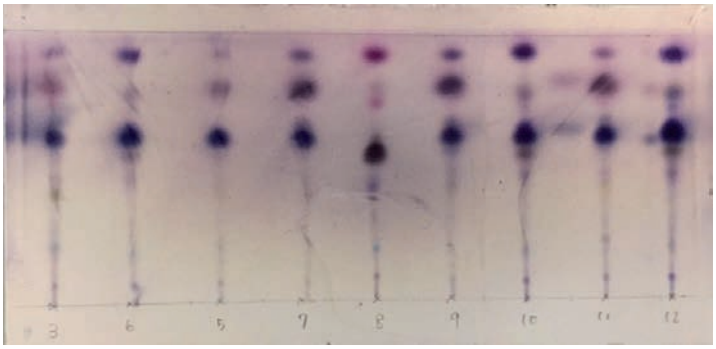
If plants are used for health benefits, or as plant-based medicines, then a difference in chemical composition will impact on the range and intensity of health-promoting effects. Plants that are physically similar can be chemically different and therefore have a different therapeutic effect. Each plant effectively has a unique chemical fingerprint.

The basil plant, *O. basilicum*

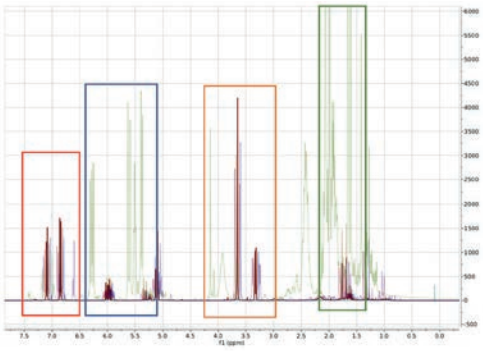
In this project, we examined the chemical composition of a range of *O. basilicum* and *O. sanctum* oils that we sourced over the internet. We used thin-layer chromatography (TLC), gas chromatography linked to mass spectrometry (GC–MS), and nuclear magnetic resonance (NMR) to compare the chemical components of nine different oils that originated in different growing areas.

Our research showed that chemical composition of the oils is very variable, depending on the place of cultivation and method of extraction. It indicates the chemical fingerprint of natural materials can be affected by cultivation, climate, soil, harvesting and storage. Therefore, it is necessary to have analytical methods that can ensure standardised products for pharmaceutical use.

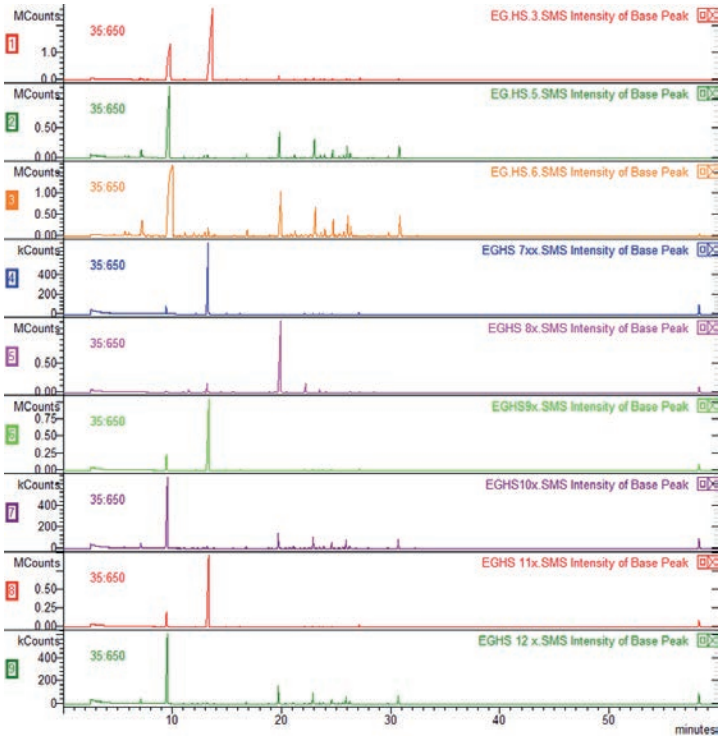
TLC plate showing the chemical differences between the nine commercial oil samples



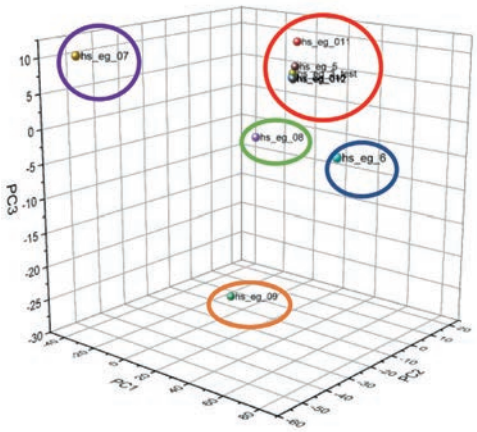
NMR data of nine essential oils present in *O. basilicum* to use as a 'reference' with key peaks highlighted



GC-MS chromatograms of basil samples from different areas of the world to compare major peaks



3D plot constructed using the NMR data from B to identify that the outlier samples (HS7 and HS9) in the batch



Results from several analytical chemistry techniques used to determine the factors that affect plant growth and influence the chemicals made by plants. Comparison against nine commercial oil samples present in *O. basilicum* to identify unique chemical fingerprints.

Thinking and discussion questions

1 If plants all have unique chemical fingerprints, how might this affect the future of medicine?

2 What other industries could benefit from the types of research Helen produces?

3 What would you do if your devices suddenly had the ability to conduct the types of high-tech instrumentation process we have looked at and could give you analysed results at the touch of a button?

Master's in pharmaceutical science

Two of **Helen's** students at Trinity College Dublin share with us how this work has influenced their careers in analytical chemistry.

Ellen Gilmartin

I am a fourth-year pharmacy student, enrolled in the five-year MPharm programme. I recently received my fourth-year results and will be graduating with a BSc in the autumn. In September, I will progress into the fifth year of the MPharm programme, and hopefully graduate as a pharmacist in autumn 2020.

In 2014, I was studying business for my Leaving Certificate and realised it wasn't for me. I decided to make a last-minute change to chemistry at the end of my fifth year. I learnt the two-year chemistry course in one year, and from there I decided I wanted to pursue a career in the area.

I also had an interest in health and wellness and so pharmacy seemed like a great way to combine all my interests. For the past four years at Trinity, I've enjoyed studying a wide range of subjects such as pharmacology, biochemistry, pharmaceutics and natural sources of drugs. I have an interest in natural products and believe that many of our major health concerns could be improved through lifestyle changes, mainly diet.

My fourth-year research project studying the properties of basil oil with Helen, was well suited to me. The genus *Ocimum* proved to be very interesting and has many proven medicinal benefits in Ayurvedic medicine. The results of this research showed the varying chemical composition of basil plants and reinforced the importance of cultivation conditions and how such conditions affect basil plant composition and biological effect.

I've been working in a community pharmacy for three years now and I really enjoy interacting and helping patients. I undertook my fourth-year placement in a pharmaceutical company and whilst it was completely different to the community setting, it touched on many other interesting areas of pharmacy that one does not come across in the clinical setting. Going forward, the future looks bright and I'm excited as to where my pharmacy career may take me.

Megumi Kitamura

I am a visiting student from Japan studying for my master's degree in pharmaceutical science, specialising in natural product chemistry. I previously studied synthetic organic chemistry of natural products in the faculty of chemical engineering.

While I was researching synthesis, I became more interested in natural products themselves. I changed my major to pharmaceutical science to focus on natural products that are used as traditional medicine. I selected this research about *Ocimum* species because it is known that they have many pharmacological activities, but there are still unexplained things about the plant and its genus.

This study has revealed some new findings related to changes in chemical composition in *O. basilicum* that come from different sources. There is great potential in studying the chemical composition of natural products, from plants and fungi to marine species. I have read some scientific journals that say we have researched only 15% of all natural plants. I really think we can study them to improve the lives of human beings. I want to be a researcher who can be a part of creating medicine for people without any remedy against their illness.

These days, biology-based medical products and regenerative medicine are becoming popular, but I believe natural materials still have enough potential for discovery of new medicines and as complementary treatments. What I learnt from this project relating to *Ocimum* and basil is the fact that the compositions of natural products are complex and variable.

These things matter in terms of when the best time might be to harvest a medicinal plant, eg opium poppies for the isolation of morphine. I got a job as a pharmaceutical researcher for a Japanese pharmaceutical company. My experience at Trinity College Dublin was a big advantage for me.

REVEALING FLAVOUR PROFILES
Food analysis 4

Cian Moloney is an advanced analytical manager at Glanbia Ireland, the largest milk producer in Ireland. He discusses his work there and a previous role as a food science specialist at Nestle Research and Development. He tells us about how he uses a variety of instrumentations to analyse and characterise the flavour profiles of products.

It is critical that we understand how our ingredients and products behave, so that we can ensure they will always meet our customers' high expectations. In my current role, I provide specialised analytical support to the team and wider business, utilising techniques such as chromatography, electrophoresis, calorimetry and rheology to build scientific knowledge of our range.

When you think about chemistry, your mind doesn't usually jump to food but, for me, food chemistry is the perfect way to bring theory to life and solve real-world problems!

Mass spectrometry

Mass spectrometry (MS) is sometimes thought of as a single technique, but in reality it describes a range of techniques that are based on a common principle. In MS, analyte molecules are first ionised, which then allows them to be separated in a magnetic or electric field based on their mass-to-charge ratio (m/z).

Only molecules of the selected m/z will reach the detector, making MS a powerful detection technique. However, there are many different methods of ionisation and means of separating analytes of different m/z, with particular instruments more suited to certain applications.

To further enhance the power of MS, it is often coupled with a separation system to perform an initial sample separation before then analysing in detail with MS – usually gas chromatography (GC) or liquid chromatography (LC). In conjunction with GC and LC, MS can be used to analyse food products to support product development and ensure quality and safety. Two such examples for infant formula are described below: GC-MS to characterise the flavour profile and LC-MS to quantify proteins.

Automated sample injector for GC-MS which can be used to analyse food samples

GC-MS

Food sensory analysis is the use of the human senses to objectively analyse foods – for properties such as taste, flavour and texture. It is used in assessing the quality of products, troubleshooting problems and new product development.

Describing the taste of a food in a scientific way that can be interpreted by others, and then using this to improve product quality in some way, is a valuable tool. Despite the many benefits of sensory analysis, it can be time-consuming, expensive and, most importantly, subjective if the panel are not trained.

Some of the common sensory defects and complaints associated with infant formula include fishy flavour and odour, paint-like, metallic taste and sulfur flavour.

Like us, each food product has its own fingerprint in the form of a typical chemical profile. It is possible to determine this fingerprint through the use of analytical instrumentation.

MS coupled with GC is very useful for the identification of chemicals responsible for off-flavours in foods and beverages. MS is generally the preferred detection method in aroma analysis, and various sampling techniques for aroma isolation and concentration can be combined with GC-MS, making it suitable for a wide range of foods and flavour compounds.

The headspace analysis sampling technique is popular due to minimal sample treatment, which reduces artefact volatile formation. Several headspace sampling techniques are available, such as static headspace, dynamic headspace, direct thermal desorption, and solid phase micro-extraction (SPME).

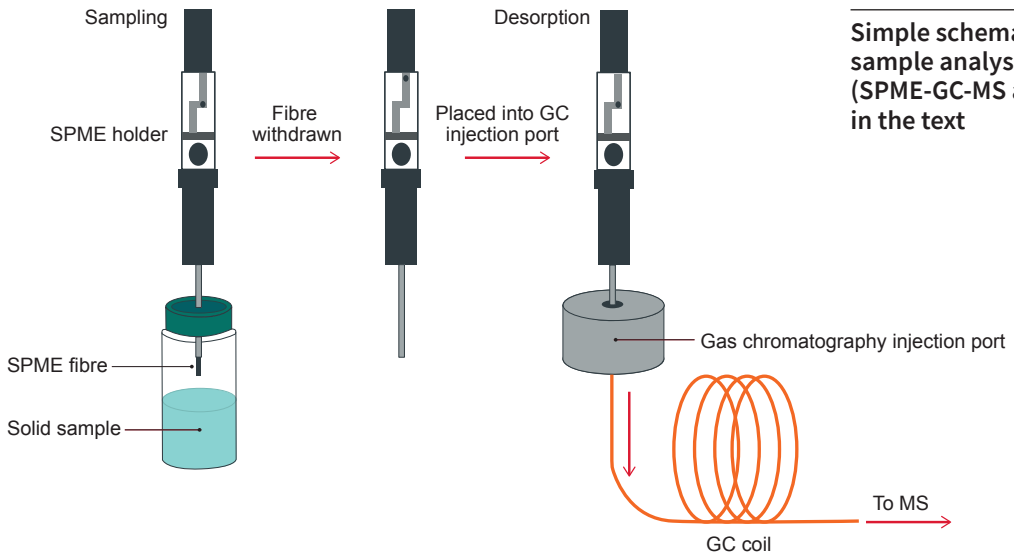
At Nestle, they characterise products using SPME-GC-MS. In SPME analysis, a spoon of infant formula is weighed and added to the sample vial, which is gently heated (~37°C) and agitated to mimic flavour release in the mouth. The volatile compounds bind to the SPME fibre in the headspace, and are later then desorbed to the GC column where they are separated, ionised and detected by the MS.

Following this analysis, the software produces a chromatogram, which we analyse using different MS libraries. What we can find from these results are a wide range of compounds being identified from aldehydes, ketones, acids, furans, esters and sulfur compounds. From the compounds identified, we can make predictions on the sensory characteristics of the infant formula analysed.

For example, if we were to detect 1-penten-3-ol (an omega-3 fatty acid oxidative degradation product), and 3,5-octadiene-2-one (related to a fishy malodour in oxidised microalgae oil and DHA powder) we can assume the infant formula will have a fishy flavour and odour.

Similarly, nonanal (linked to volatile oxidation products of fish oils) can impart a paint-like, grassy flavour and therefore is definitely not a compound we want to find in our products!

The results from trained sensory panels are cross-referenced against the GC-MS data using statistical analyses to develop models and further confirm that if the compounds detected in the product are imparting the expected flavours and aromas in real-world settings.



Simple schematic depicting sample analysis using (SPME-GC-MS as described in the text

LC-MS

Proteins are important nutritional components of milk and infant formula and methods to measure the protein content of milk have been available for well over 100 years. However, while measurement of total protein is readily achievable, the quantification of individual proteins (for example, those of particular nutritional interest) can be challenging. High performance liquid chromatography or electrophoresis can be used, but in many cases it is very difficult to separate proteins with similar structures or sizes, and proteins present at low levels can be difficult to detect at all. Further complicating matters, many milk proteins are expressed as a range of genetic variants, each with its own structure.

LC-MS can be used to bypass many of these issues, allowing us to identify and quantify individual proteins with high accuracy and confidence. To achieve this, instead of trying to detect the entire protein, we digest the protein with an enzyme, and then detect and measure signature peptides that could come only from the protein of interest. It is much easier to quantify relatively small peptides, compared to large proteins that are prone to side-reactions and whose behaviour is generally less predictable.

In LC-MS, we first use LC to separate the sample components (as well as determining the retention time of the target peptide, which helps to confirm the analyte identity). The sample elutes from the LC instrument and is directly transferred to the triple-quadrupole MS, where it is ionised. Next, the ions are pulled under vacuum into the mass filter (in our case, a quadrupole), where the charges on the poles are precisely set so that only ions of our peptide m/z should have a stable trajectory to successfully make it to the other end of the quadrupole.

To make the technique even more specific, the ions then enter a collision cell where they are fragmented by a stream of inert nitrogen gas.

The fragments are sent to a second quadrupole where only fragments of a specified m/z should make it to the end.

LC-MS used in analysis laboratories

Thinking and discussion questions

1 Why is it important to be able to identify small compounds with high accuracy and confidence?

2 Discuss the idea of using instrumentation instead of people to conduct food analysis.

UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

Elizabeth Gilchrist, a lecturer in analytical chemistry at the school of chemistry and environmental research Institute, University College Cork, tells us about how mass spectrometry is frequently used in forensic science to confidently identify what is in a sample collected at a crime scene.

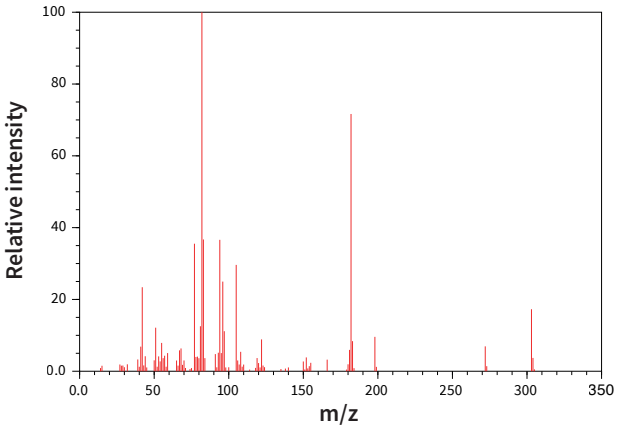
Mass spectrometry (MS) can be used on its own, or it can be combined with other chemical analysis techniques, such as liquid chromatography (LC), to provide powerful separation and identification capabilities.

Some interesting forensic applications of MS include:

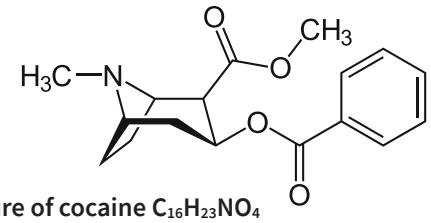
- debris from arson or explosive incidences. We don't expect the compounds of interest to be in large quantities and MS is sensitive enough for trace analysis. Important evidence in these cases includes accelerants (ie petrol) or explosive residues (ie TNT);
- tissue samples or bodily fluids, such as blood and sweat. This can inform us whether an individual has taken drugs, poisons or alcohol. This area is known as toxicology and can include drink driving, performance-enhancing drugs taken by athletes, as well as monitoring drug use or establishing cause of death;
- recently, MS imaging has been used to obtain fingermark ridge detail simultaneously with the distribution of illicit compounds, such as explosives and drugs, that have been handled by the perpetrator. This allows the potential to link identity with criminal activity;
- drug analysis is a huge area in forensics – there are thousands of drug seizures annually in Ireland, and it is important to confirm whether the suspect material seized is illicit or not, as well as how pure the sample is.

Often packages containing suspect controlled drugs are seized. They are usually in the form of a white powder and as such undergo confirmatory testing using LC-MS. These results (shown below) conclude the molecule to be cocaine.

Garda National Drugs Unit tested 217 cocaine samples between April 2010 and March 2012. It found that the average purity of cocaine was between 15 and 19%. The highest purity was 68%, the lowest just 0.2%. Street samples are regularly cut with adulterants to make it look like there's more cocaine than there is. These can sometimes be substitutes that give similar effects to cocaine but at a lower cost, such as benzocaine, lidocaine or procaine, sometimes other drugs such as caffeine or paracetamol, but also boric acid, tetramisole hydrochloride (used to treat worms in animals), dimethylterepthalate (used to make plastic films), and even laundry detergent.



Mass spectrum of cocaine



Structure of cocaine $C_{16}H_{23}NO_4$

Thinking and discussion questions

1 What are the implications of a purity level that changes between 68% and 0.2%?

2 Why is it useful to be able to use MS along with other techniques such as liquid chromatography?

Quantative chemistry ideas

- Moles calculations
- Teaching moles from first principles
- Student support sheets
- Titration calculations
- Titrations vs instrumentation
- Applied questions

MOLES CALCULATIONS
The triangle method

Edith Kearney at Lusk Community College is one of our teacher members and she provided us with these teaching strategies for mole calculations.

To calculate any one of three unknowns in the formula triangle (pictured), mass, moles or relative atomic mass (Ram), simply cover the one you want to know and use the relationship between the other two to calculate the unknown quantity. If the relationship between the other two is one above or below the other; then you use division, ie number of moles = mass/Ram. If the two knowns are side by side, then multiply them to find the unknown, ie mass = number of moles × Ram.

Example: If you want to know the mass of 1 mole of baking soda, then cover the mass symbol in the formula triangle. You would then use the mole(s) and Ram to calculate the mass.

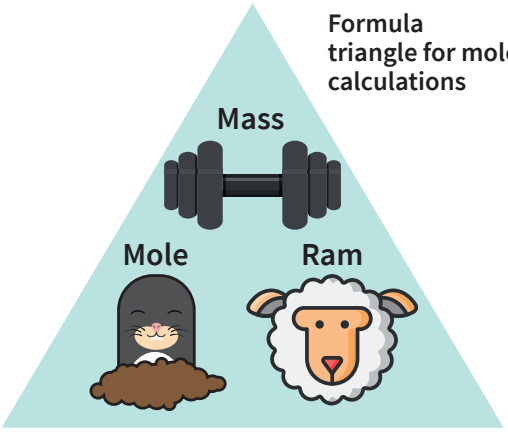
First use the RAM of each atom to calculate the relative molecular mass for baking soda Na2HCO3):

relative molecular mass = 23 + 1 + 12 + (16 × 3) = 84

Then, multiple the number of moles by the relative molecular mass to get the mass:

Mass = 1 mole × 84 = 84 g

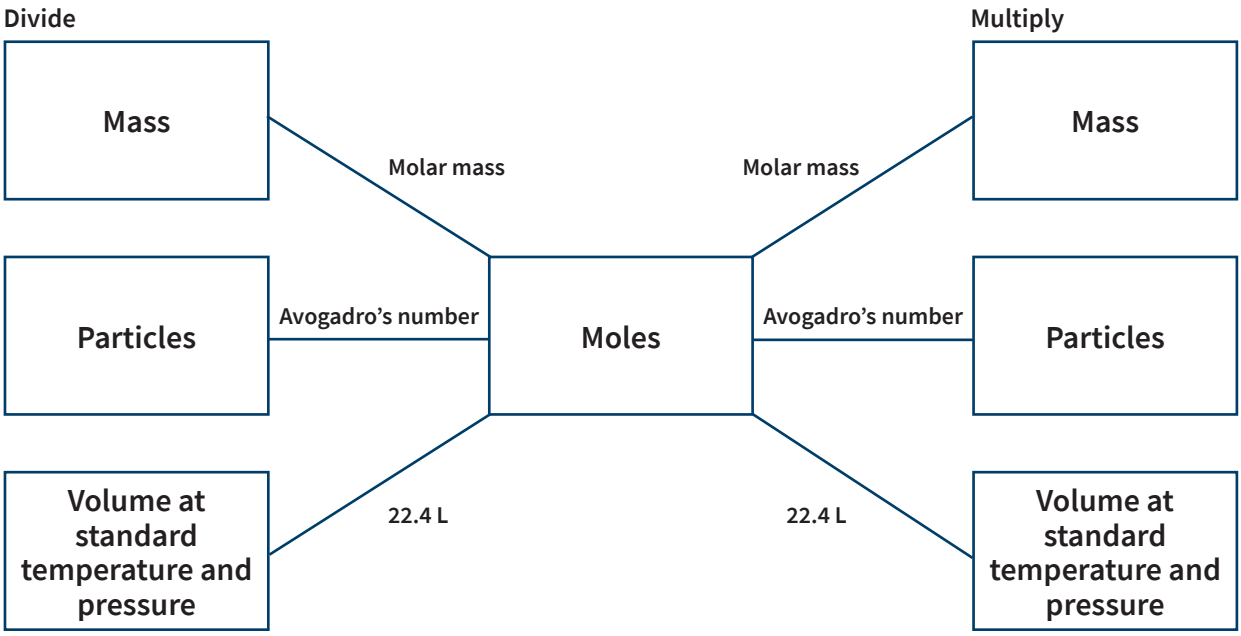
1 mole of baking soda weighs 84 g.



Formula triangle for mole calculations

Divide and multiply grid

Going from left to right, divide boxes and lines to get the middle box, and going further right, multiply the middle box by the lines to get the ones in the far right boxes.



Example: If I have 6.02×10^{23} particles of sodium how many moles of sodium do I have?

6.02 × 1023 (number of particles)
6.02 × 1023 (Avogadro's number)
= 1 mole sodium

STUDENT SUPPORT SHEET ONE
Teaching moles from first principles

What is a mole?

It is a representation of a really big number of tiny particles.

In the same way that a dozen represents 12, 1 mole is actually 6.02×10^{23} atoms. This big number is known as Avogadro's number, after the scientist who discovered it.

In chemistry, we can't weigh out such small quantities and measure them, so scientists use the mole. A mole of a substance refers to a quantity, like a dozen eggs means 12. A mole of hydrogen means there are 6.02×10^{23} atoms of hydrogen.

If 1 mole of carbon has 6.02×10^{23} atoms, and we can't weigh the tiny particles, then we need to know how much 1 mole weighs. Conveniently, scientists do know how much 1 mole weighs for each element, and so do you … look no further than the periodic table.

This is why if we know the relative atomic mass (Ram or Ar) of something from the periodic table we can calculate the moles!

What is a titration?

Titrations are used by chemists when amounts of particles (that we can't see) are being used to measure the amount of particles in another solution (that we also can't see).

Chemists do this in a slow and controlled way using titration equipment, until they know the chemical reaction is complete. They use an indicator to show when this has happened, known as the end point – this is usually a colour change.

'First principles' method of calculating the unknown

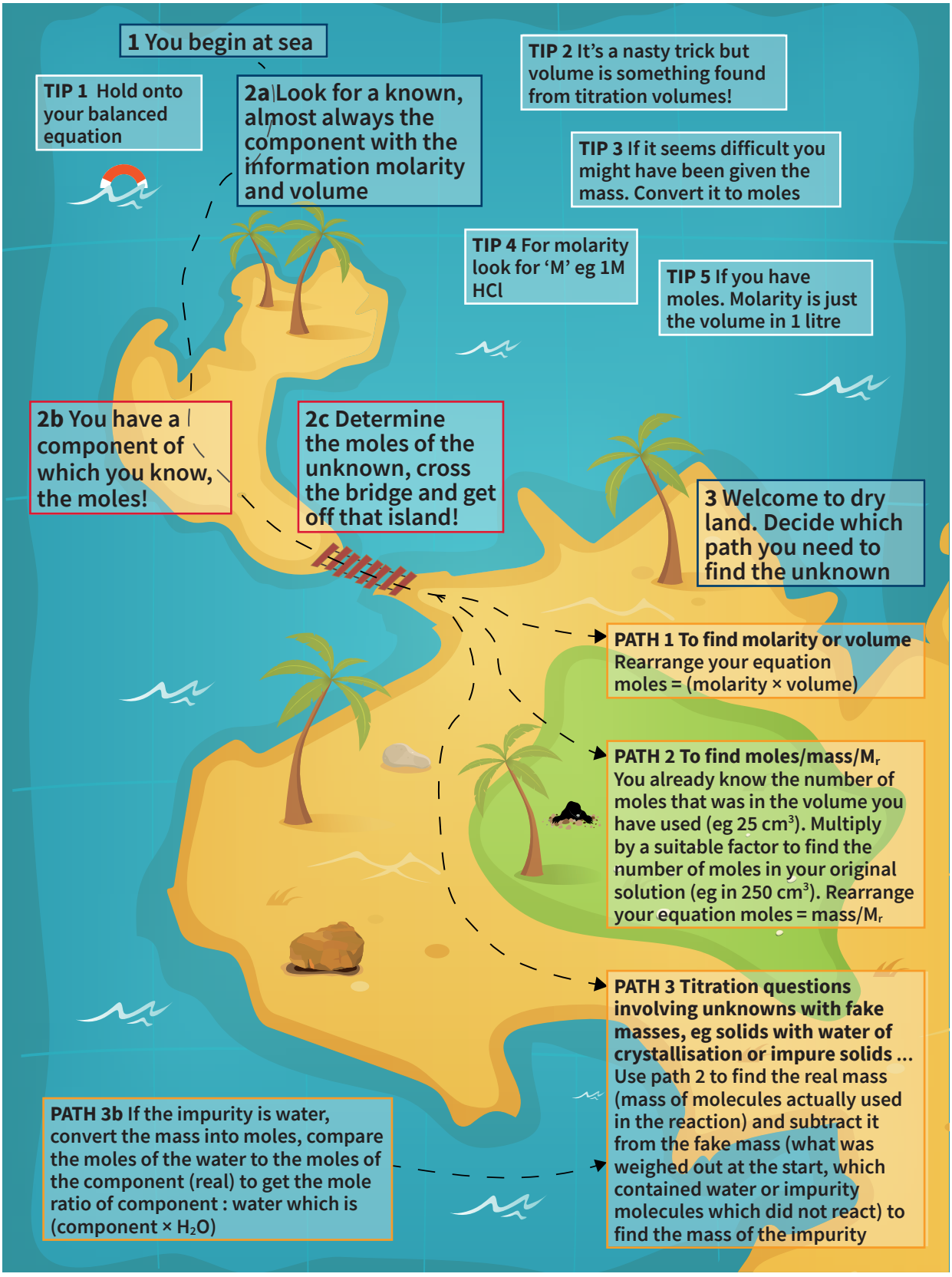
Chemists can also calculate the unknown from first principles, ie find out the number of moles of one reactant and, knowing the mole ratio of reaction, find out the moles of the other. The following equations apply.

1 moles = mass/M_r Note: M_r is the relative molecular mass

2 moles = (molarity × volume)/1000

Titration island analogy

The map below might help you to begin to navigate exam titration problems. There are a few guided problems that you can use to get the hang of the map. Then you can try and find your own way through for the unguided questions.



Titration island analogy – guided example one

Start

1 Find the balanced equation and therefore mole ratio:

$$1HCl + 1NaOH \rightarrow 1NaCl + 1H_2O$$

2a Look for the molarity and volume; this is known for HCl.

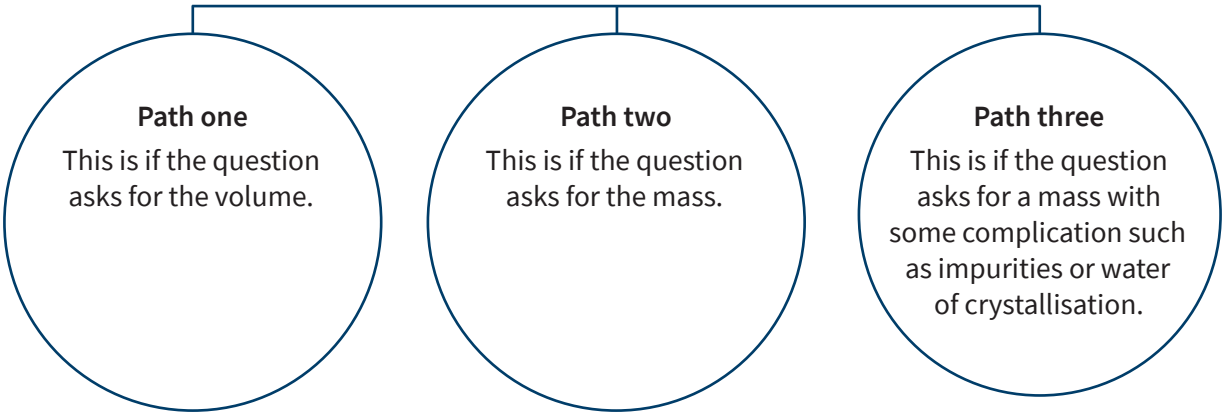
2b Calculate the number of moles of HCl = $\frac{\text{molarity} \times \text{volume}}{1000}$

moles = 27.2 × 0.1/1000
Therefore 0.00272 moles HCl was used in the titration

2c Use the mole ratio to establish the moles of the unknown that was used in the titration.
0.00272 moles HCl was used, therefore 0.00272 moles NaOH was used in the titration.

Path choices

Then take the correct path:



Path two

This example asks for moles, and moles = mass/relative molecular mass

We know that the number of moles that was in the 25 cm^3 of NaOH used in the titration was 0.00272. Therefore the moles that would be in the original 250 cm^3 solution would be this multiplied by 10.

0.00272 × 10 = 0.0272 moles in 250 cm^3
Since moles = mass/M_r 0.0272= ×/40

Rearranging this gives 0.0272 × 40 = 1.088 g of NaOH in the original solution.

Titration island analogy – guided example two

Finding the formula of a compound

Sodium carbonate crystals (15.7 g) were dissolved in water and made up to 1 litre. A 25.0 cm^3 portion of the solution was neutralised by 26.5 cm^3 of 0.1 M hydrochloric acid solution.
What is *x* in $Na_2CO_3.xH_2O$?

$$Na_2CO_3 + 2HCl \rightarrow 2NaCl + H_2O + CO_2$$

Start

1 Establish the mole ratio* of reactants

*the *x* in $Na_2CO_3.xH_2O$ is also a mole ratio but it isn't relevant to the titration part.

Mole ratio
$1Na_2CO_3 : 2HCl$

2a Establish the known:

HCl is the known

2b Establish the number of moles of the known:

Moles of HCl used in the reaction = 26.5 × 0.1/1000 = 0.00265

2c Calculate the moles of the unknown used in the reaction:

Using the mole ratio to calculate the number of moles of sodium carbonate that reacted
0.00265/2 = 0.001325 moles Na_2CO_3 reacted

Make path choices

Path three because it is an impure or fake mass.

0.001325 moles Na_2CO_3 were used in the reaction, and therefore this is how many moles of Na_2CO_3 were present in the 25 cm^3 portion of $Na_2CO_3.xH_2O$ solution.

The 25 cm^3 came from 1 L of original solution (x40).

Therefore (x40) = 0.053 moles of Na_2CO_3 were in the original solution.

The original question tells us that the fake mass used to make the solution was 15.7 g

What was the real mass (ie the mass of Na_2CO_3 in the solid that was used to make the original solution)?

0.053 moles = mass/M_r (106)

Therefore the mass of Na_2CO_3 used to make the original solution was 5.618 g.

Of the 15.7 g used to make the original solution, only 5.618 g was Na_2CO_3 and the rest of the mass was water (10.08 g water).

Because moles = mass/M_r (18 for water) the number of moles of water in 10.08 g = 0.55 moles.
Mole ratio 0.053 Na_2CO_3 : 0.55 H_2O (simplify to 1 : 10).

Therefore the formula is: $Na_2CO_3 : 10H_2O$ and *x* = 10

STUDENT SUPPORT SHEET TWO
Vinegar titration in detail from first principles

Vinegar is a mild acid. Its chemical name is ethanoic acid and its formula is CH_3COOH. Shop-bought vinegar is usually a mixture of this acid plus water and flavouring agents.

To determine the concentration of ethanoic acid in a sample of vinegar, 20.0 cm^3 of the vinegar was diluted up to 100 cm^3 in a volumetric flask and then the diluted vinegar was titrated with a standard solution of sodium hydroxide.

The standard solution contained 1.20 g of sodium hydroxide in 500 cm^3 of solution.

On average, 14.0 cm^3 of the diluted vinegar was required to neutralise 25.0 cm^3 of this sodium hydroxide solution.

The equation for the titration reaction is:

$$CH_3COOH + NaOH \rightarrow CH_3COONa + H_2O$$

Calculate:

1 The number of moles of sodium hydroxide in each 25.0 cm^3 portion

2 The number of moles of ethanoic acid per cm^3 of diluted vinegar

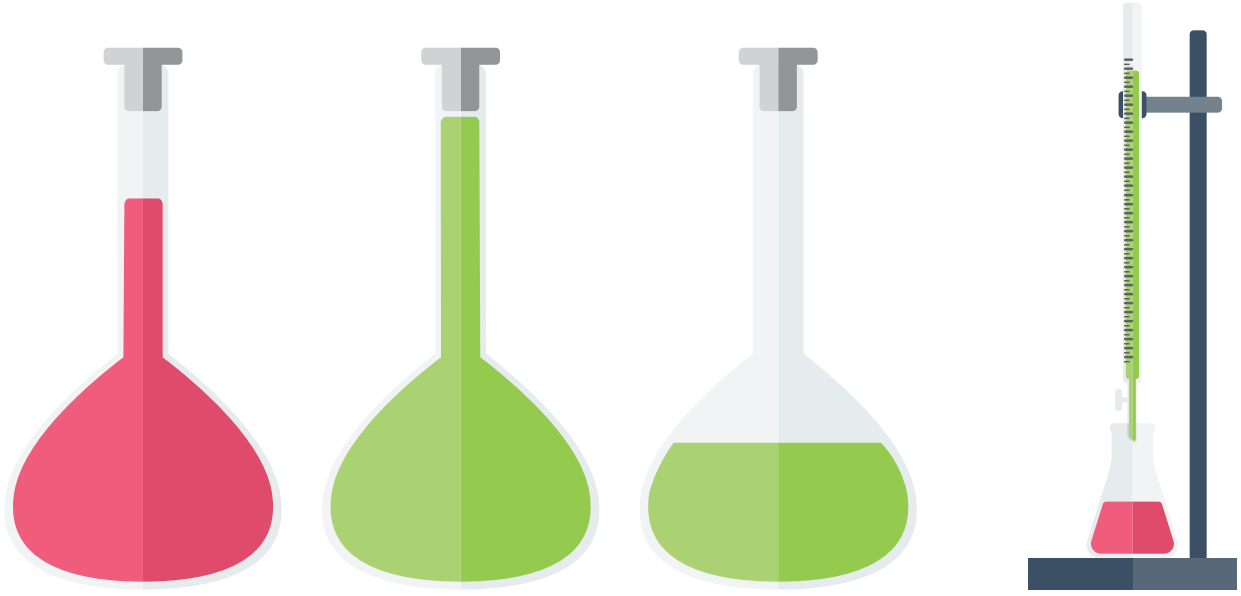
Find the concentration of ethanoic acid in the original vinegar:

3 In terms of moles per litre

4 As a percentage (weight per volume: w/v)

First identify and label your reagents from the selection below. Identify which solution goes into the burette and which into the conical flask, using colour to reflect your choice.

- 500 cm^3 of a standard solution of sodium hydroxide
- Burette and conical flask
- 100 cm^3 of diluted vinegar
- 20 cm^3 of vinegar

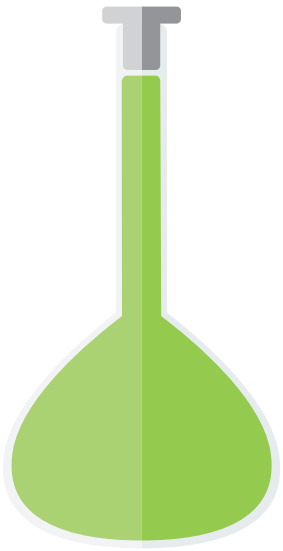


Suggested practical set-up for the vinegar titration

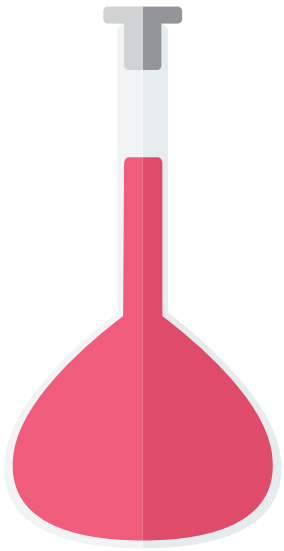
Vinegar titration in detail from first principles (continued)

1 Work out what you know

CH_3COOH + $NaOH$ → CH_3COONa + H_2O



Unknown concentration
20 cm^3 in 100 cm^3 = dilution factor of five



Unknown concentration

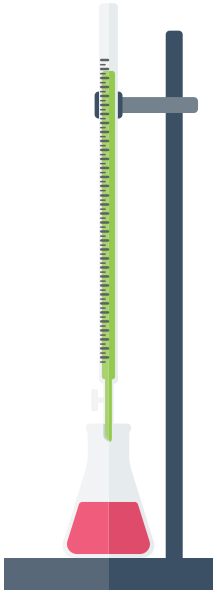
1.20 g of sodium hydroxide in 500 cm^3 = 2.4 g of sodium hydroxide in 1 L

To find moles use:

moles = mass/M_r

2.4 g ÷ 40 = 0.06 M

The reaction between acetic acid and sodium hydroxide



The unknown always goes in the burette

2 Use moles of known to find moles of unknown

Find the number of moles in the known (sodium hydroxide in 25 cm^3) to work out the moles of the unknown concentration (diluted vinegar).

1 Apply the equation number of moles = $\frac{\text{molarity} \times \text{volume}}{1000}$

Molarity: 0.06
Volume: 25.0 cm^3

number of moles = $\frac{0.06 \times 25.0}{1000}$ = 0.0015 moles

2 **Use the molar ratio** to relate the known mole quantity to the unknown number of moles. The balanced equation tells us they react in a ratio of 1:1, in this case we can say that 0.0015 moles of NaOH reacts with 0.0015 moles of vinegar. We can use this number of moles to calculate the molarity of the diluted vinegar.

= 0.0015 moles in 25 cm^3

$NaOH$

0.0015 moles in 14.0 cm^3

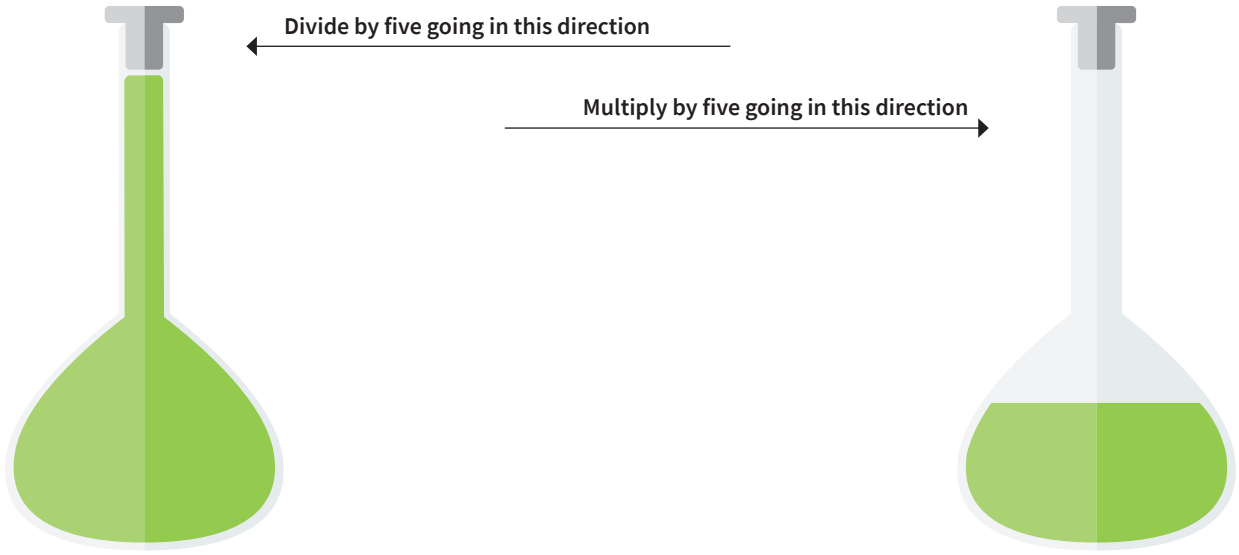
CH_3COONa

$\frac{0.0015}{14} \times 1000 = 0.107$ M

Volume: 14 cm^3
molarity: ?

3 Look at the dilution factor

Find the concentration of the original vinegar in mol/L … The vinegar was diluted by a factor of five.



Molarity of the diluted sample of vinegar = 0.107 M

Hence the molarity of the original sample of vinegar 0.107 M × 5 = 0.535 M

4 Change to appropriate units

Find the concentration of the original vinegar in g/L and in % w/v.

The concentration of ethanoic acid in the original vinegar sample in g/L:

1 We find the M_r of ethanoic acid

CH_3COOH

$[M_r = 12 + 3(1) + 12 + 2(16) + 1 = 40]$

2 Apply the equation 0.535 mol/L × 40 = 21.4 g/L

3 Finally, to find the % w/v, ie g/100 cm^3

4 21.4/10 = 2.14 g/100 cm^3

The concentration of ethanoic acid in vinegar is 2.14% w/v

STUDENT SUPPORT SHEET THREE
Quantifying

Remember!

Concentration – the amount of a solute that is dissolved in a known volume solution

Solute – the substance that is dissolved

Solvent – the liquid that does the dissolving

Solution – the mixture of solute and solvent

Units

- Percentage (%) of solute (weight per weight, weight per volume, or volume per volume)
- Parts per million (ppm)
- Molarity (moles per litre)

Percentage of solute (weight per weight: w/w)

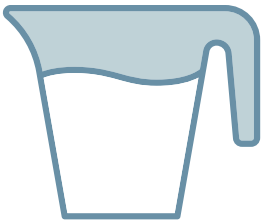
i 5 g of salt mixed with a powder until 50 g is reached

ii 5 g/50 g = 0.1 g

iii 0.1 × 100 = 10% solution

1 I am preparing a specific tablet for a patient with an allergy to one of the normal ingredients. I mix 2 g of the active ingredient with 10 g of lactose before I put it in the tablet compressor. What is my w/w%?

Percentage of solute (weight per volume: w/v)



i 5 g of salt dissolved in water and adding water until a total weight of 50 g of solution is reached (use a balance).

ii Calculate the % concentration

iii 5 g/50 g = 0.1 g/g (this means for every 1 g of water you will find 0.1 g of dissolved salt)

iv 0.1 × 100 = 10% solution

2 A parent asks for paracetamol suspension for a very small baby. I don't have that concentration in stock so I must make it up, it needs to be 120 mg/5 ml. What is its w/v%?

Percentage of a liquid dissolved in a liquid (volume per volume: v/v)

i 5 cm^3 of ethanol added to water. Water is added until the total volume reaches 50 cm^3.

ii 5 cm^3/50 cm^3 = 0.1 cm^3/cm^3 (in 1 cm^3 of water you will find 0.1 cm^3 of ethanol)

iii 0.1 × 100 = 10% solution

3 You need to make a mouthwash and you use a base alcohol solution which is labelled as 10% v/v. How much alcohol is in 200 cm^3?

Parts per million (ppm)

Used when the concentration of a solution is very dilute. It presents when 1 mg of a substance is dissolved in 1 litre (1000 cm^3) of solution, ie milligrams per litre (mg/L).

i Convert 100 cm^3 into litres (L) 1L = 1000 cm^3 100/1000 = 0.1L

ii Convert 0.02 g into mg. 1000 mg = 1 g 1000 × 0.02 = 20 mg

iii You have 20 mg/0.1L =200 ppm (200 mg per litre)

4 Fluoride tablets should not be given to patients if fluoride in the water supply exceeds 0.7 ppm (this is the same as saying 0.7 mg/L). If the concentration of fluoride where your patient lives is 0.25 ppm, how many litres would have 1 mg of fluoride?

5 How much fluoride is the patient consuming in a day? The average person drinks 2 litres of water per day.

Molarity (moles of solute per litre)

Molarity is the number of moles of a solute per 1 litre of solution. A 1 molar (1 M) solution contains 1 mole of solute per 1 litre of solution.

Moles of a substance is calculated using the equation: moles = mass / M_r .

Example: If you have 2 moles in a litre then you have a molarity of 2 M, or half a mole per litre is 0.5 M.

Answers

1 20% w/w

2 2.4% w/v

3 20 cm^3

4 0.25 ppm = 0.25 mg/L (therefore 4 litres would be needed to make 1 mg)

5 0.5 ppm

TITRATION VERSUS INSTRUMENTATION
Comparing methods

John O'Donoghue is based in the school of chemistry at Trinity College Dublin. He divides his time between the university and the Royal Society of Chemistry as an education coordinator. He was the project coordinator in Ireland for Spectroscopy in a Suitcase, which was funded by Science Foundation Ireland (SFI) and the Royal Society of Chemistry. He has provided the following teaching resource to support teachers in titration versus instrumentation.

When chlorine compounds are used to sterilise swimming pool water, the active agent is usually chloric(I) acid, HOCl. It kills micro-organisms by oxidation. Chloric(I) acid and its conjugate base, the chlorate(I) ion, ClO^-, together make up what is called 'free chlorine'. These species react with a solution of iodide ions in the same way as chlorine itself does. When chlorine reacts with potassium iodide in an acidic solution it liberates iodine:

$$Cl_2 + 2KI \rightarrow I_2 + 2KCl$$

The intensity of the colour of the iodine solution formed is a measure of the concentration of the oxidising chlorine in water. The concentration of chlorine in a sample of swimming pool water or diluted bleach is obtained by comparing the colour obtained on reaction with potassium iodide solution with those colours obtained by the similar reactions of some standard solutions of chlorine.

Safety considerations:
(Goggles must be worn. The use of gloves is recommended)

- Dilute ethanoic acid is slightly corrosive.
- Potassium iodide is an irritant.
- Domestic bleach is an irritant.

Procedure

1 Add 2.5 cm^3 of Milton sterilising fluid to a 250 cm^3 volumetric flask and dilute to the mark with deionised water to make a 100-fold dilution (final concentration will be 200 mg/L or 200 ppm).

2 To a series of five 100 cm^3 volumetric flasks add 5 cm^3 of 5% ethanoic acid solution.

3 Accurately add the appropriate amount of the Milton solution to make a serial dilution of standards.

4 Add 5 cm^3 of 2% potassium iodide solution to each flask (including the blank) and dilute to the mark with deionised water. Stopper each flask, mix thoroughly, and allow about 5 minutes for the colour to develop.

5 Switch on the colorimeter and choose the correct wavelength filter (400 nm). Use the blank sample to zero the instrument before starting any other measurement. Use the correct setting for this.

6 Pour each working standard into a cuvette, rinsing each cuvette first with the solution it is to contain.

7 Obtain the absorbance for each standard, using the run/collect sample absorbance feature.

8 Plot a graph of absorbance versus concentration for the series of standards.

9 Unknown sample: to a 100 cm^3 volumetric flask add 5 cm^3 of 5% ethanoic acid solution, and then 5 cm^3 of 5% potassium iodide solution. Fill the flask up to the mark with the swimming pool water or diluted bleach to make the unknown sample. Allow about 5 minutes for the colour to develop.

10 Obtain the absorbance for the unknown solution and using the graph calculate the concentration of NaOCl in the sample.

Disposal of wastes:

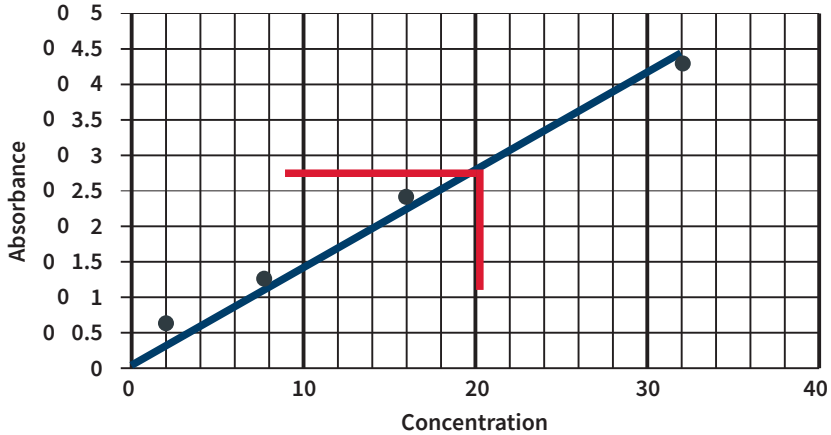
Add 1 M sodium thiosulfate solution to the waste to neutralise. When colourless, dilute with water and flush to foul water drain.

CHEMICAL	BLANK	FLASK A	FLASK B	FLASK C	FLASK D	UNKNOWN
5% ethanoic acid	5 cm^3	5 cm^3	5 cm^3	5 cm^3	5 cm^3	5 cm^3
2% potassium iodide	5 cm^3	5 cm^3	5 cm^3	5 cm^3	5 cm^3	5 cm^3
Diluted Milton bleach	0 cm^3	1 cm^3	2 cm^3	3 cm^3	4 cm^3	Swimming pool water
Total flask volume using deionised water	100 cm^3	100 cm^3	100 cm^3	100 cm^3	100 cm^3	100 cm^3
Conc NaOCl (ppm) (x-axis)	0	2	4	6	8	?
Absorbance from colorimeter (y-axis)	0					

Background information and notes

- For swimming pool water, the operation must be carried out within a short period of time of taking the sample from the pool. The level of free chlorine drops rapidly as it reacts with organic matter in the sample, so any delay would result in an inaccurate reading.
- Most of the time for this experiment is in making up the working standards. Only one colorimeter is needed for a class, as colorimeter readings can be taken very quickly.
- The blank must be run first and is usually a different button than the sample button on the colorimeter.
- The cuvettes need to be rinsed out with deionised water immediately after use, as otherwise they will become coloured by the iodine.
- The concentration of free chlorine (in the form of OCl^-, and expressed as Cl_2) is found by multiplying by 51.5/74.5, as this is the ratio of the molar mass of Cl_2 to that of NaOCl.
- Milton sterilising fluid is used because it contains a 2% sodium hypochlorite solution. If left unopened after purchasing until the day of the experiment, it should be very satisfactory. The diluted solution has a sodium hypochlorite concentration of approximately 200 mg per litre.

Absorbance versus concentration of NaOCl



If your colorimeter only gives transmittance you can convert to absorbance as here. For further reference see sigmaaldrich.com/technical-documents/articles/biology/transmittance-to-absorbance.html

Example results and calculations:

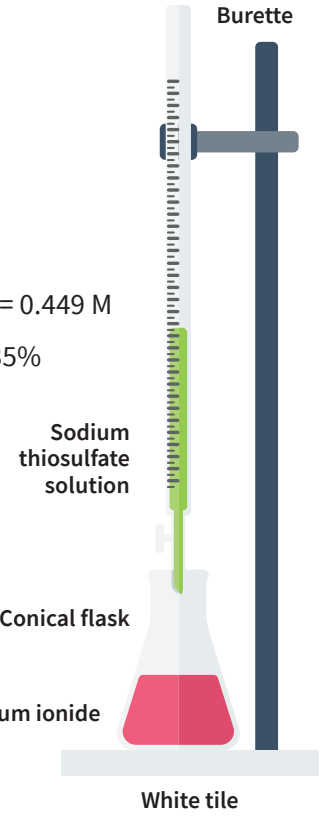
Absorbance blank	= 0.00
Absorbance of solution in flask A	= 0.06
Absorbance of solution in flask B	= 0.12
Absorbance of solution in flask C	= 0.24
Absorbance of solution in flask D	= 0.43
Absorbance of unknown solution	= 0.18
Concentration of NaOCl in the sample	= 12.6 ppm (from graph)
Concentration of free chlorine in the sample	= 8.71 ppm

Iodine/thiosulfate titration:

- We can also determine the percentage (w/v) of sodium hypochlorite in household bleach or swimming pool water via titration. Instead of a 100-fold dilution used for the colorimetry experiment, a 10-fold dilution of the bleach is used here.
- Most household bleaches contain hypochlorite salts such as sodium hypochlorite (NaOCl).

  $ClO^- + 2I^- + 2H^+ \rightarrow Cl^- + I_2 + H_2O$
- Liberated iodine can be titrated against sodium thiosulfate.
- Starch indicator added when the solution in the conical flask turns straw yellow.
- Continued until solution goes from blue-black to colourless.

  $I_2 + 2S_2O_3^{2-} \rightarrow 2I^- \rightarrow 2I + S_4O_6^{2-}$
- Volume of thiosulfate solution used = 22.45 cm^3
- Moles of thiosulfate used = 22.45 × 0.1/1000 = 0.002245 moles
- Balanced equations: $ClO^- : S_2O_3^{2-} = 1 : 2$
- Moles of hypochlorite solution used = 0.002245/2 = 0.0011225 moles
- Moles/cm^3 of hypochlorite solution = 0.0011225/25 = 0.0000449
- Moles/litre of hypochlorite solution = 0.0449
- Concentration of hypochlorite in diluted bleach solutions = 0.0449 M
- Concentration of hypochlorite in undiluted bleach solution = 0.0449 × 10 = 0.449 M
- Percentage (w/v) of hypochlorite (NaOCl) in bleach = 74.5 × 0.449/10 = 3.35%
- Remember 1% = 10,000 ppm
- Flask = 25 ml bleach (diluted by 10×), 1 g KI, 10 cm^3 H_2SO_4



Applied questions

The following section contains a variety of questions, some based on skills learnt from the different projects and some set in the context of a careers story.

1 The accepted value is 25.35. Tick which correctly describes this student's experimental data.

Trial	Measurement
1	25.48
2	24.97
3	25.27

a accurate but not precise ☐
b precise but not accurate ☐
c both accurate and precise ☐
d neither accurate nor precise ☐

2 The accepted value is 2.43. Tick which correctly describes this student's experimental data.

Trial	Measurement
1	2.29
2	2.93
3	1.88

a accurate but not precise ☐
b precise but not accurate ☐
c both accurate and precise ☐
d neither accurate nor precise ☐

3 The accepted value is 15.63. Tick which correctly describes this student's experimental data.

Trial	Measurement
1	12.84
2	13.02
3	19.96

a accurate but not precise ☐
b precise but not accurate ☐
c both accurate and precise ☐
d neither accurate nor precise ☐

APPLIED QUESTIONS
Titration calculations

To determine the concentration of thiosulfate solution a student titrates the unknown against 25 cm^3 of a standard solution of iodine. The student added 5.08 g of iodine to the 500 cm^3 volumetric flask to make the standard solution.

1 Calculate the concentration (in moles per litre) of thiosulfate when 19.55 titres were required to reduce the 25 cm^3 of iodine.

$$I_2 + 2S_2O_3^{2-} \rightarrow S_4O_6^{2-} + 2I^-$$

a Calculate the moles of iodine in the standard solution.

b Calculate the moles of iodine in the 25 cm^3 portions.

c Using the ratio calculate how many moles of S_2O_3 react with the iodine.

d Calculate the concentration in moles per litre of the thiosulfate.

2 A sample of hydrated sodium carbonate crystals was made up to 250 cm^3 in a volumetric flask, and 25 cm^3 of the resultant solution was reacted with 0.1 M HCl with the average titre giving a reading of 20.5.

$$2HCl + Na_2CO_3 \rightarrow NaCl + H_2O + CO_2$$

a Calculate the moles per litre.

b Calculate the grams per litre of the washing soda.

3 2.15 g of hydrated ethanedioic acid, $H_2C_2O_4.nH_2O$, were dissolved in distilled water and the solution made up to 250 cm^3 in a graduated flask. Then 25.0 cm^3 of this solution were titrated by 17 cm^3 of 0.200 mol dm^{-3} NaOH(aq). How many molecules of water of crystallisation are there in the hydrated ethanedioic acid? H = 1; C = 12; O = 16.

$$H_2C_2O_4 + 2NaOH \rightarrow Na_2C_2O_4 + 2H_2O$$

APPLIED QUESTIONS
Answers

Applied questions

1 A – accurate but not precise.

2 C – both accurate and precise.

3 B – precise but not accurate.

Titration questions

1 a Number of moles (n) = mass (m)/relative molecular mass (M_r)
$n = 5.08 \times 2/254 = 0.04$ moles per litre

b $n = C \times V/1000$ $n = 0.04 \times 25/1000 = 0.001$

c 1 : 2 0.001 : 0.0005

d $n = C \times V/1000$ $0.0005 = ? \times 19.55/1000$
$C = 0.026$ units mol/L

2 a $C1 \times V1 = C2 \times V2$ $? \times 25 = 0.1 \times 20.5$ $? = 0.082$
Divided by the ratio $0.082/2 = 0.041$

b $n = \text{mass}/M_r$
$0.041 = x/106$
$x = 4.34$ g

3 $H_2C_2O_4 + 2NaOH \rightarrow Na_2C_2O_4 + 2H_2O$
$H_2C_2O_4$: NaOH is 1 : 2

Moles NaOH = $17 \times 0.2/1000 = 0.0034$

Moles $H_2C_2O_4 = 0.0034/2 = 0.0017$ per 25 cm^3

Times by 10 in 250 = 0.017

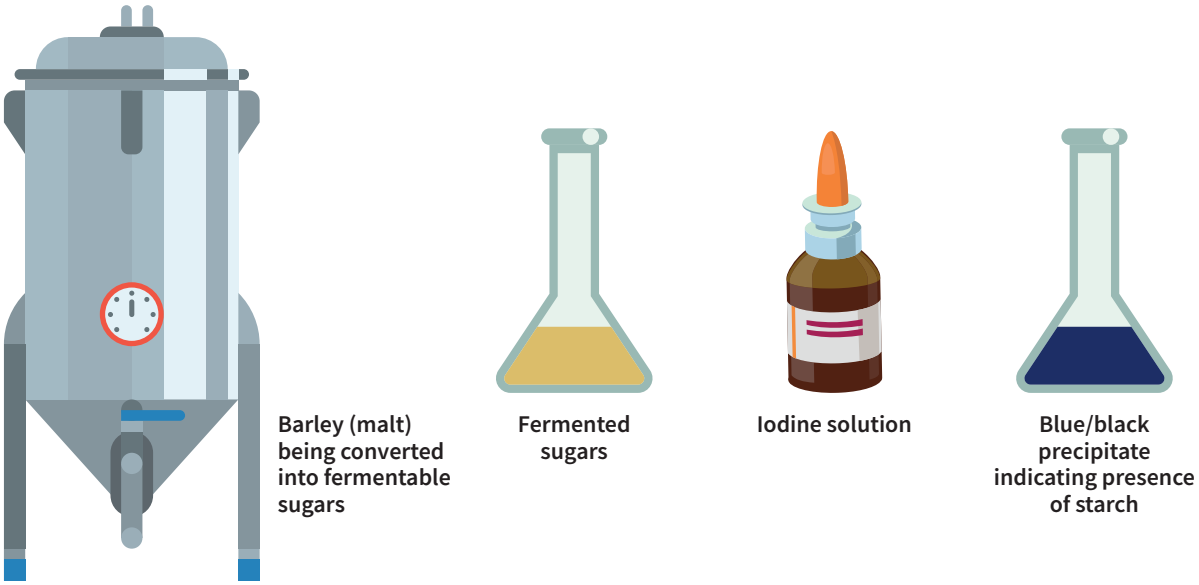
So, 2.15 g of $H_2C_2O_4.nH_2O$ is 0.017 moles
$n = \text{mass}/M_r$ $0.017 = 2.15/x$ $x = 2.15/0.017$
$x = 126$

So $(2 \times 1) + (2 \times 12) + (4 \times 16) + 18n = 126$
$90 + 18n = 126$
$n = 2$

Cathal Connolly from Alltech tell us about how their work uses titrations and instrumentation

Typically, analysis at Alltech uses much more sophisticated instrumentation than titration. However, there is one titration that is exceedingly useful as it allows us to get results quickly and accurately. We use the starch iodine reaction both qualitatively and quantitatively.

Qualitatively we will use it in brewing scenarios, eg to test whether all of the starch from the barley (malt) has been converted into fermentable sugars so that the yeast can metabolise it into alcohol (ethanol) and carbon dioxide during fermentation.



A brief outline of the apparatus for a 'by eye' starch test

This test involves a sample being taken from the tank and brought to the lab for a quick visual test following addition of a few drops of iodine (Lugol's solution). The formation of a black precipitate indicates the presence of starch, so the enzymatic hydrolysis reactions might need more time for completion.

Quantitatively we use titrations for carrying out enzyme assays (ie we will check on how active our enzyme has been at breaking down the starch).

Initially we will use the enzyme to hydrolyse (break down the chemical bonds) in our starch substrate (turning it into glucose) and then do a back-titration using sodium thiosulfate to quantify the amount of starch that still remains.

The qualitative and quantitative analysis Cathal talks about includes various ways of detecting concentration, some more rigorous than others. The 'by eye' test Cathal performs is a crude qualitative test often used by scientists to check if the process is working as expected; he also might be able to make some assumptions about the concentration. To generate more conclusive quantitative results for how actively the enzymes have been breaking down the starch he can measure it in two ways – a back-titration or colorimetry.

Method one, using a back-titration

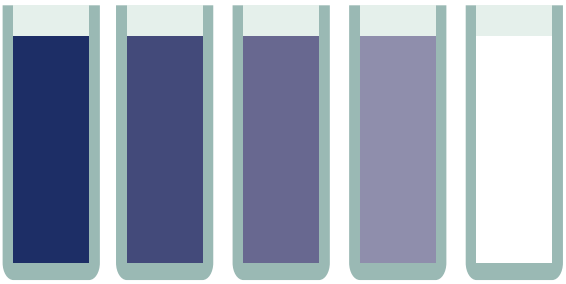
Cathal takes a sample of the hydrolysed material, containing mostly glucose and the remaining starch. The concentration of starch can be analysed by a back-titration with an iodine solution (they react in a 1 : 1 ratio). He adds 2 moles of excess iodine solution to the leftover starch, and dilutes the solution to 250cm^3 stock solution, of which 25 cm^3 aliquots react with 0.1 moles of sodium thiosulfate.

$$I_2 + 2S_2O_3^{2-} \rightarrow S_4O_6^{2-} + 2I^-$$

1 Calculate the moles of the starch left over from the enzyme assay.

Secondly, using colorimetry

For the calibration curve Cathal makes 50 cm^3 of a 1% solution of starch in distilled water, and he then makes serial dilutions until he has six different concentrations. To each he adds one drop of iodine solution. He transfers each of these solutions into the cuvettes for the colorimeter.



Starch and iodine solutions of increasing dilution used to make the calibration curve

He includes a blank cuvette in his sample then proceeds to read the absorbance of the seven cuvettes at 'orange' wavelengths (610 nm).[1] These are his results:

Starch concentration (%)	Average absorbance (orange 610 nm)
1	1.078
0.7	0.966
0.5	0.91
0.3	0.708
0.1	0.517
0.05	0.436
0	0

Affix graph here

Using the graph help sheet, produce the graph for Cathal and use it to work out the unknown concentration.

References

1 Results taken from **nuffieldfoundation.org/practical-biology/making-calibration-curve-starch-concentration**

1 Graph analysis (four marks)

2 Putting the unknown starch solution in the colorimeter gives an absorbance of 0.9. What was the concentration of this solution?

HL questions:

3 Why was a blank used?

4 Are these results quantitative or qualitative? Explain.

5 Why was orange light used?

Extension activity

Probe your knowledge of this topic and instrumentation by exploring the simulation **edu.rsc.org/resources/beers-law-simulation/1432.article**

1 Describe what happens to the absorption when you increase the concentration.

2 Clicking on the double-sided yellow arrow to make the beaker as big as it can be, adjust the concentration and read the absorbance. Do this for four different concentrations. Sketch a graph of this relationship.

Click on variable wavelength (just below the light beam).

a Which has a higher wavelength, blue or red?

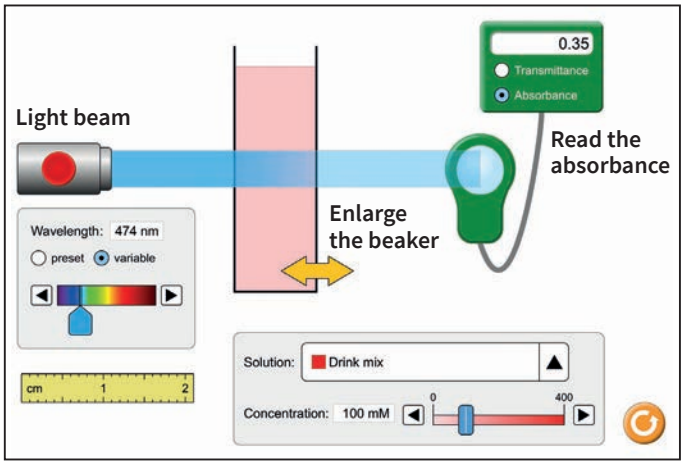
b Try a blue wavelength with a blue drink. What happens to the absorbance?

c **HL** Why does this happen?

Consider Beer's law: $A = \varepsilon C \ell$ (A = absorbance, ε = molar absorptivity, C = concentration and ℓ = path length).

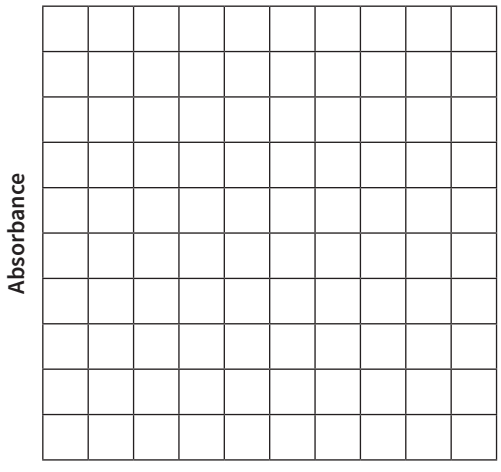
3 Investigating this relationship, try and achieve the highest value for absorbance and then lowest. What did you do differently each time?

Beer's law simulation



edu.rsc.org/resources/beers-law-simulation/1432.article

Calibration curve graph



Graph axes for the calibration curve to show the relationship between absorbance and concentration

Applied back-titration

Answer – using the three steps from the previous analogy.

1 Excess iodine solution – starch = unreacted iodine

2 Unreacted iodine 1 : 2 sodium thiosulfate
Moles of S_2O_3 = 0.1
Moles of unreacted iodine = 0.05
Moles × 10 = initial unreacted iodine = 5 moles

3 Excess iodine solution – starch = unreacted iodine
2 moles – 0.5 moles = 1.5 moles of starch

Calibration curve

Graph analysis

1 As concentration increases, the absorbance of light at this wavelength is also increasing (one mark). Give two values (two marks).

Explaining the theory – a higher concentration means more molecules, therefore there are more molecules absorbing the light, so the absorbance is higher at higher concentrations (one mark).

2 About 0.5.

3 To check the machine is functioning and calibrated.

4 Quantitative
For qualitative data, analysis of the data can usually be done from the table of results as this requires making observations and the inferences from the observations.

For quantitative data, analysis involves collecting numerical values, using this to carry out calculations or presenting the numerical values in a graph to establish a relationship between independent and dependent variables or to find an unknown value.

5 Orange light was used because the solution is blue and therefore will reflect blue light, and its complementary will be absorbed (orange).

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p13 Nuclei flipping magnetic spin, after I Hunt, NMR Spectroscopy, University of Calgary, Department of Chemistry **chem.ucalgary.ca/courses/350/Carey5th/Ch13/ch13-nmr-1.html**

p13 1H NMR spectrum image, source: G Rocchitta and P Serra, OA Alcohol, 2013, 1, DOI: 10.13172/2053-0285-1-2-840

p16 Image © Shutterstock

Project 1 Emission competition

p23 Images © Jerry Zhu, from **cs.cmu.edu/~zhuxj/astro/html/spectrometer.html**

p24 Emission spectrum from a sodium street lamp **spectralworkbench.org/spectrums/56511**, uploaded on August 21, 2015 23:08 UTC CC-BY-SA 2017 @ ncanever and other Public Lab contributors

p26 Prism refracting visible light spectrum © Science Photo Library C023/0219

pp26–27 Spectra images sourced from 'Build a spectroscope' activity **solar-center.stanford.edu**, accessed March 2020 and reproduced under © 1996–2015 by the Stanford SOLAR Center, Solar Observatories Group, Stanford University, CA

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p31 Emission spectra image © iStock/Getty Images Plus

p31 Emission spectrum from a sodium street lamp, **spectralworkbench.org/spectrums/56511**, uploaded on August 21, 2015 23:08 UTC CC-BY-SA 2017@ncanever and other Public Lab contributors

Project 2 Phone-y science

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Project 3 Building a mass spectrometer

p63–67 This activity has been inspired by and adapted from Rosie Research's Making a Mass Spectrometer, **rosieresearch.com/making-mass-spectrometer**

p75 Graph shows the mass spectrum produced for a sample of boron, after **chemguide.co.uk/analysis/masspec/elements.html#top**

Project 4 The sunshine factor

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