Maths for Chemists

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Foreword

Mathematics is an essential and integral component of all of the scientific disciplines, and its applications within chemistry are numerous and widespread. Mathematics allows a chemist to understand a range of important concepts, model physical scenarios, and solve problems. In your pre-university studies it is likely you have already encountered the use of mathematics within chemistry, for example the use of ratios in mixing solutions and making dilutions or the use of logarithms in understanding the pH scale. As you move through your university studies you will see mathematics increasingly used to explain chemistry concepts in more sophisticated ways, for example the use of vectors in understanding the structures of crystals, or numerical approximations of ordinary differential equations (ODEs) in kinetics to predict the rates and mechanisms of chemical reactions. The ability to understand and apply mathematics will be important regardless of the branch of chemistry you are studying, be it the more traditional areas of inorganic, organic and physical chemistry or some of the newer areas of the subject such as biochemistry, analytical and environmental chemistry.

For some time it has become apparent that many students struggle with their mathematical skills and knowledge as they make the transition to university in a wide range of subjects. From our own experiences of teaching undergraduates we have been aware of this 'mathematics problem' in chemistry and in 2014 we commenced a research project, working with four excellent and highly motivated undergraduate summer interns, to try to reach a better understanding of these issues. We also wanted are and to develop materials and resources to aid learners as they begin their study of chemistry within higher education. At the University of Leeds educational research was undertaken to analyse existing data sets and capture the views and opinions of both staff and students; the findings of this work were then used by student interns at the University of Birmingham to develop this guide.

There are already a range of textbooks available that aim to help chemistry students develop their mathematical knowledge and skills. This guide is not intended to replace those, or indeed the notes provided by your lecturers and tutors, but instead it provides an additional source of material presented in a quick reference style allowing you to explore key mathematical ideas quickly and succinctly. Its structure is mapped to include the key mathematical content most chemistry students encounter during the early stages of their first year of undergraduate study. Its key feature is that it contains numerous examples demonstrating how the mathematics you will learn is applied directly within a chemistry context. Perhaps most significantly, it has been developed by students for students, and is based upon findings from the research undertaken by students.

While this guide can act as a very useful reference resource, it is essential you work to not only understand the mathematical ideas and concepts it contains, but that you also practice your mathematical skills throughout your undergraduate studies. Whereas some people adopt what might be termed a 'formulaic approach', following a structured process of applying particular formulae or equations to a problem, this will not work all of the time and the reasons why might be quite subtle. Understanding key mathematical ideas and being able to apply these to problems in chemistry is an essential part of being a competent and successful chemist, be that within research, industry or academia.

With even a basic understanding of some of the mathematics that will be used in your chemistry course, you will be well prepared to deal with the concepts and theories of chemistry. We hope this guide provides a helpful introduction to mathematics as you begin your study of chemistry within higher education. Enjoy, and good luck!

Michael Grove, Joe Kyle & Samantha Pugh
September 2014

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0 Introduction

We have made this booklet to assist first year chemistry students with the maths content of their course. It has been designed as an interactive resource to compliment lecture material with particular focus on the application of maths in chemistry. We have produced this booklet using resources, such as lecture notes, lecture slides and past papers, provided to us by the University of Birmingham and the University of Leeds.

0.1 About the Authors

Allan Cunningham is in his fourth and final year of an MSci Mathematics degree at the University of Birmingham. His dissertation is on the topic of Positional Games in Combinatorics.

Rory Whelan is currently in his second year of a joint honours course in Theoretical Physics and Applied Mathematics at the University of Birmingham. When he isn't doing physics or maths he enjoys juggling and solving Rubik's cubes.

0.2 How to use this Booklet

- The contents contains hyper-links to the sections and subsections listed and they can be easily viewed by clicking on them.
- The book on the bottom of each page will return you to the contents when clicked. Try it out for yourself now:
- In the booklet important equations and relations appear in oval boxes, as shown below:

$$\boxed{\text{Chemistry} > \text{Maths}}$$

- Worked examples of the mathematics contained in this booklet are in the blue boxes as shown below:

Example: What is the sum $1 + 1$?

Solution: $1 + 1 = 2$

- Worked chemistry examples that explain the application of mathematics in a chemistry related problem are in the yellow boxes as shown below:

Chemistry Example: What is the molecular mass of water?

Solution: The molecular formula for water is H_2O. We have that the atomic mass of oxygen is 16 and hydrogen is 1. Hence the molecular mass of water is equal to $16 + (1 \times 2) = 18$.

- Some examples can also be viewed as video examples. They have hyper-links that will take you to the webpage the video is hosted on. Try this out for yourself now by clicking on the link below:

Chemistry Example: An ion is moving through a magnetic field. After a time t the ion's velocity has increased from u to v. The acceleration is a and is described by the equation $v = u + at$. Rearrange the equation to make a the subject.

Click here for a video example

Solution: ...

1 Mathematical Foundations

1.1 Addition, Subtraction, Multiplication and Division

We will all be familiar with the following operations: addition ($+$), subtraction ($-$), multiplication ($\times$) and division ($\div$) but for the sake of completeness we will review some simple rules and conventions.

Operator	Representation	Ordering
Addition	$A + B$	$A + B = B + A$
Subtraction	$A - B$	$A - B \neq B - A$
Multiplication	$A \times B$ or $A \cdot B$ or $A * B$ or AB	$A \times B = B \times A$
Division	$A \div B$ or $\frac{A}{B}$	$\frac{A}{B} \neq \frac{B}{A}$

Addition and Multiplication are Distributive

For numbers x, y and a the distributive rule for addition and multiplication is:

$$\boxed{a \times (x + y) = (a \times x) + (a \times y)}$$

Example:
For example suppose we have $x = 3$, $y = 5$ and $a = 6$ then:

1. $a \times (x + y) = 6 \times (3 + 5) = 6 \times 8 = 48$
2. $(a \times x) + (a \times y) = (6 \times 3) + (6 \times 5) = 18 + 30 = 48$

So $a \times (x + y) = (a \times x) + (a \times y)$ and the distributive rule holds.

Factorisation

Factorisation is used to tidy up equations in order to make them easier to read and understand.

Example:
We can factorise the equation $y = 8x + 12$ if we note that both $8x$ and 12 are divisible by 4 this gives us $y = 4(2x + 3)$.

Note: It is mathematical convention not to include the $\times$ symbol when multiplying so $4x$ means $4 \times x$ and in the above example $y = 4(2x + 3)$ means $y = 4 \times (2x + 3)$.

Example:
We can factorise the equation $y = 3x^3 + 6x$ if we note that both $3x^3$ and $6x$ are divisible by $3x$ this gives us $y = 3x(x^2 + 2)$.

Multiplying Out Terms

Multiplying out terms (or expanding out of brackets) makes use of the distributive law to remove brackets from an equation and is the opposite of factorisation.

Example:
We can multiply out the equation $y = 5(x + 3)$ to give $y = (5 \times x) + (5 \times 3) = 5x + 15$.

Example:
We can multiply out the equation $y = 3z(2x^4 + 7)$ to give:

$$y = (3z \times 2x^4) + (3z \times 7)$$
$$\implies y = 6zx^4 + 21z$$

Example:
We can multiply out the equation $3a[(a + 3b) - 5(2b - a)]$ to give: $3a[(a + 3b) - (5 \times 2b - 5 \times a)]$
$= 3a[(a + 3b) - (10b - 5a)]$

$= 3a(6a - 7b)$

$= 18a^2 - 21ab$

Adding and Subtracting Negative Numbers

1. Adding a negative number is like subtracting a positive number.
2. Subtracting a negative number is like adding a positive number.

Example:
Suppose we have $x = 4$ and $y = -3$.

$$x + y = 4 + (-3) = 4 - 3 = 1$$
$$x - y = 4 - (-3) = 4 + 3 = 7$$

Order of Operations: BODMAS

Consider the calculation below:

$$6 + (7 \times 3^2 + 1)$$

In what order should we calculate our operations? BODMAS tells us that we should carry out the operations in the order listed below:

1. First Brackets.
2. Then Orders. (This is the powers and roots).
3. Then Division.
4. Then Multiplication.
5. Then Addition.
6. Then Subtraction.

Note: Addition and subtraction have the same priority so can actually be done in either order. The same is true for multipication and division.

Example:
So returning back to $6 + (7 \times 3^2 + 1)$

$6 + (7 \times 3^2 + 1)$	Start inside the Brackets and do the Orders first
$6 + (7 \times 9 + 1)$	Then Multiply the 7 and 9
$6 + (63 + 1)$	Then Add the 63 and 1
$6 + (64)$	Brackets are done so the last operation is to Add the 6 and 64
70	

Chemistry Example: Calculate the molecular mass of $CuSO_4 \cdot 5\,H_2O$ hydrated copper sulphate.

Solution:

$$\begin{aligned}
\text{Molecular mass of } CuSO_4 \cdot 5\,H_2O &= 64 + 32 + (16 \times 4) + 5 \times ((1 \times 2) + 16) \\
&= 64 + 32 + 64 + 5 \times (2 + 16) \\
&= 64 + 32 + 64 + 5 \times 18 \\
&= 64 + 32 + 64 + 90 \\
&= 250
\end{aligned}$$

Chemistry Example: Below is the van der Waals equation:

$$\left(p + \frac{an^2}{V^2}\right)(V - nb) = nRT$$

which relates the pressure p, the volume V and the absolute temperature T of an amount n of a gas where a and b are constants.

Suppose we have 1.0 mol of argon gas occupying a volume of 25×10^{-3} m^3 at a pressure of 1.0×10^5 Pa and $a = 0.10$ Pa m^6 mol^{-2} and $b = 4.0 \times 10^{-5}$ m^3 mol^{-1}. Calculate the left hand side of the equation.

Solution: Using BODMAS we start with the brackets. In this question we have two brackets so we begin with the first of them on the left side by substituting the values from the question:

$$\begin{aligned}
\left(p + \frac{an^2}{V^2}\right) &= \left(1 \times 10^5 + \frac{0.1 \times 1^2}{(25 \times 10^{-3})^2}\right) && \text{Do the Orders} \\
&= \left(1 \times 10^5 + \frac{0.1 \times 1}{625 \times 10^{-6}}\right) && \text{Then Divide and Multiply} \\
&= (1 \times 10^5 + 160) && \text{Then finally Add} \\
&= 1.0016 \times 10^5
\end{aligned}$$

We now calculate the second bracket. First substitute the values from the question:

$$\begin{aligned}
(V - nb) &= (25 \times 10^{-3} - 1 \times 4 \times 10^{-5}) && \text{Then Multiply} \\
&= (25 \times 10^{-3} - 4 \times 10^{-5}) && \text{Then Subtract} \\
&= 2.496 \times 10^{-2}
\end{aligned}$$

Finally as both brackets have been calculated we can find their product.

$$\left(p + \frac{an^2}{V^2}\right)(V - nb) = 1.0016 \times 10^5 \times 2.496 \times 10^{-2} = 2.5 \times 10^3 \text{ Pa m}^3 \text{ to 2 significant figures.}$$

1.2 Mathematical Notation, Symbols and Operators

In order to save ourselves time we often use symbols as shorthand. We look at three new symbols Δ, Σ and Π which are used to describe operations, just like $(+)$, $(-)$, $(\times)$ and $(\div)$.

The Delta Δ Operator

We use the Greek capital letter Δ (called delta) to represent the difference (or change) between the start and end values of a quantity. For any quantity A:

$$\Delta A = A_{\text{final}} - A_{\text{initial}}$$

where A_{final} is the final amount of A and A_{initial} is the initial amount of A so ΔA is equal to the difference in these two values.

Note: If ΔA is positive then there is an increase in A and if ΔA is negative then there is a decrease in A.

Chemistry Example: If the optical absorbance Abs increases from 0.65 to 1.35 during a reaction, what is $\Delta(Abs)$?

Solution: First recall that:

$$\Delta(Abs) = Abs_{\text{Final}} - Abs_{\text{Initial}}$$

From the question $Abs_{\text{Initial}} = 0.65$ and $Abs_{\text{Final}} = 1.35$. Hence $\Delta(Abs) = 1.35 - 0.65 = 0.70$.

The Sigma Σ Operator

The Greek capital letter Σ (called sigma) is used to represent a sum, normally long sums which would take a while to write out completely. The general form for a sum using sigma is:

$$\sum_{i=1}^{n} X_i = X_1 + X_2 + X_3 + \cdots + X_n$$

Below we have what each of the terms in the sum means:

- X_i are the numbers that are being summed; it could be an expression involving i.
- i is called the summation index; it identifies each term in the sum.
- $i = 1$ tells us to start summing at $i = 1$.
- n tells us to stop summing when we have reached $i = n$.

For a numerical explanation, consider take the sum $1+2+3+4+5$. This can be simplified into the sum notation as $\sum_{i=1}^{5} i$. From the notation we can see that we are summing the number i from when i is equal to 1 to 5.

Example: What is the value of $\sum_{i=4}^{7} i^2$

Solution: To begin we 'read' what the operation is telling us to do. We know it is a sum from the Σ and the terms we are summing are the squares of the index. We are starting with 4 and ending at 7 (and assume that each number is an integer). This then will give us:

$$\sum_{i=4}^{7} i^2 = 4^2 + 5^2 + 6^2 + 7^2 = 16 + 25 + 36 + 49 = 126$$

The summation index might not be numbers, for example when finding the RMM (relative molecular mass) of a molecule we sum the masses of all its constituent elements. This can be expressed as:

$$\sum_{i=\text{Element}} N_i M_i$$

where i goes through all the elements present in the molecule. N_i is the number of element i atoms in the molecule and M_i is the RAM (relative atomic mass) of element i.

For example finding the RMM of methane CH_4 would look like this:

$$\sum_{i=\text{Elements}} N_i M_i = N_{\text{Carbon}} M_{\text{Carbon}} + N_{\text{Hydrogen}} M_{\text{Hydrogen}} = (1 \times 12) + (4 \times 1) = 16$$

The Pi Π Operator

You will be familiar with the Greek letter π (called pi) as the constant $3.141\ldots$ But capital pi Π is used as an operator. The operation it represents is similar to the one that the Sigma operator does, but instead of adding all the terms you multiply them. The general form for the product using the Pi is:

$$\prod_{i=1}^{n} X_i = X_1 \times X_2 \times X_3 \times \cdots \times X_n$$

All the other notation you should recognise from the Sigma operator.

Note: An easy way to remember which is which, **S**igma = **S**um, **P**i = **P**roduct.

Chemistry Example: A chemist is making a species that requires 3 steps. The first step gives a 66% yield, the second gives a 50% yield and the third gives a 95% yield. What is the overall percentage yield for this synthesis?

Solution: We can calculate the overall percentage yield by using the Pi operator as the overall yield is the product of all the individual yields.

$$\text{Overall Yield} = \prod_{i=1}^{3} (\text{yield of step } i)$$

Plugging the numbers in gives:

$$\text{Overall Yield} = (\text{yield of step 1}) \times (\text{yield of step 2}) \times (\text{yield of step 3})$$
$$\text{Overall Yield} = 0.66 \times 0.50 \times 0.95 = 0.3135$$

Hence the overall percentage yield will be $0.3135 \times 100 = 31\%$ to 2 significant figures.

1.3 Fractions

Fractions are a way of expressing ratios and are synonymous to division. They are written in the form:

$$\frac{A}{B}$$

- The expression on the top of a fraction A is called the **numerator**.
- The expression on the bottom B is known as the **denominator**.

Note: Fractions are used as a nicer way of showing division ie: $a \div b = \dfrac{a}{b}$

Simplifying Fractions

Plenty of fractions can be reduced to simpler forms, for example $\frac{2}{4}$ is the same as $\frac{1}{2}$. The best way of simplifying is to find a number that is a factor of the numerator and the denominator so that it cancels.

Example: Simplify $\dfrac{350}{1000}$ into its simplest form.

Solution: We first notice that a factor of 10 can be taken out of both the numerator and denominator, leaving us with:

$$\frac{10 \times 35}{10 \times 100} = \frac{\cancel{10} \times 35}{\cancel{10} \times 100} = \frac{35}{100}$$

The only remaining factors of 35 are 7 and 5. 5 is also a factor of 100 so we can take it out as a factor as well:

$$\frac{35}{100} = \frac{5 \times 7}{5 \times 20} = \frac{\cancel{5} \times 7}{\cancel{5} \times 20} = \frac{7}{20}$$

We can not simplify any further because the numerator and denominator share no more factors.

Example: Simplify $\dfrac{2x + 6xy}{4x^2 + 10x^3}$.

Solution: We note first all the terms are even this means we can take a factor of 2 out. Also all the terms have an x in them meaning we can take a factor of x out.

Since we now have a factor of $2x$ on both the numerator and denominator it will cancel, leaving us with a fraction that can't be simplified any more. The following steps are illustrated below.

$$\frac{2x + 6xy}{4x^2 + 10x^3} = \frac{2(x + 3xy)}{2(2x^2 + 5x^3)} = \frac{2x(1 + 3y)}{2x(2x + 5x^2)} = \frac{\cancel{2x}(1 + 3y)}{\cancel{2x}(2x + 5x^2)} = \frac{1 + 3y}{2x + 5x^2}$$

Chemistry Example: What fraction of water's mass is hydrogen?

Solution: Recall the relative atomic mass of oxygen and hydrogen are 16 and 1 respectively. Remeber also that the molecular formula for water is H_2O.

So the molecular mass of water is equal to $(1 \times 2) + 16 = 18$. The mass of the hydrogen in water is 2, so out of the 18 amu (atomic mass units) 2 are of the hydrogen. Expressed as a fraction this is $\frac{2}{18}$ which simplifies to $\frac{1}{9}$.

Note: Don't fall into the trap when simplifying shown in this incorrect example:

$$\frac{a + b}{b + c} = \frac{a + \cancel{b}}{\cancel{b} + c} = \frac{a}{c} \qquad \text{WRONG!}$$

If you still are uncertain then use $a = 1, b = 2, c = 3$ and then be shocked to find that $\frac{1}{3} = \frac{3}{5}$!

Multiplying Fractions

Multiplying two fractions together is a simple process, the numerator is the product of the numerators and the denominator is the product of the denominators.

$$\boxed{\frac{a}{b} \times \frac{x}{y} = \frac{a \times x}{b \times y}}$$

Generally when we multiply many fractions together, the numerator is the product of *all* the numerators and similarly with the denominators. Using the Π notation we can generalise this as:

$$\boxed{\frac{a}{b} \times \frac{c}{d} \times \cdots \times \frac{y}{z} = \frac{a \times c \times \cdots \times y}{b \times d \times \cdots \times z} = \frac{\prod_a^y \text{numerators}}{\prod_b^z \text{denominators}}}$$

Note: If we are multiplying a fraction by a number that isn't in fraction form, such as an integer or π, then it will only multiply the numerator. We do this by treating it as a fraction in the form $\frac{\text{number}}{1}$ as shown in question 2 of the next example.

Example: Find the following:

1. $\frac{1}{2} \times \frac{2}{3} \times \frac{4}{5} \times \frac{5}{7}$
2. $5\sqrt{2} \times \frac{3}{10}$

Solution:

1. $\frac{1}{2} \times \frac{2}{3} \times \frac{4}{5} \times \frac{5}{7} = \frac{1 \times 2 \times 4 \times 5}{2 \times 3 \times 5 \times 7} = \frac{40}{210} = \frac{4}{21}$
2. $5\sqrt{2} \times \frac{3}{10} = \frac{5\sqrt{2}}{1} \times \frac{3}{10} = \frac{5\sqrt{2} \times 3}{1 \times 10} = \frac{15\sqrt{2}}{10} = \frac{3\sqrt{2}}{2}$

Chemistry Example: A chemist prepares a solution containing $\frac{1}{50}$ mole of propanol in 1000ml of water. How many moles are there in a 250ml aliquot of this solution?

Solution: To calculate this we need to know what fraction 250 ml is to 1000ml. That will be $\frac{250}{1000}$ which simplifies to $\frac{1}{4}$.

The number of moles taken out is then the product of the two fractions, $\frac{1}{50} \times \frac{1}{4} = \frac{1 \times 1}{50 \times 4} = \frac{1}{200}$.

Dividing Fractions

The inverse of the fraction is where the numerator and denominator switch, e.g. fraction $\frac{a}{b}$ has an inverse of $\frac{b}{a}$.

Division is the inverse of multiplication so when we divide by a fraction we are essentially multiplying by the inverse of that fraction. So a general example of division of fractions would look like:

$$\boxed{\frac{\left(\frac{a}{b}\right)}{\left(\frac{c}{d}\right)} = \frac{a}{b} \times \frac{d}{c} = \frac{ad}{bc}}$$

Example: Find the following:

$$\frac{9}{16} \div \frac{3}{4}$$

Solution:

$$\frac{9}{16} \div \frac{3}{4} = \frac{9}{16} \times \frac{4}{3} = \frac{9 \times 4}{16 \times 3} = \frac{36}{48} = \frac{3}{4}$$

Adding and Subtracting Fractions

To be able to add and subtract two fractions they both need to have the same denominator called a 'common denominator'. Take $\frac{1}{4} + \frac{1}{5}$ for example. We need a new denominator for both in order to add them. The easiest denominator to pick is almost always the product of the two so in this case $4 \times 5 = 20$.

$$\frac{1}{4} + \frac{1}{5} = \left(\frac{1}{4} \times \frac{5}{5}\right) + \left(\frac{1}{5} \times \frac{4}{4}\right) = \frac{5}{20} + \frac{4}{20} = \frac{9}{20}$$

Subtracting fractions works exactly the same way, the denominators need to be the same but you then subtract at the end.

Example: Find $\dfrac{1}{3} + \dfrac{1}{6}$. Express your answer as a simplified fraction.

Solution: The first thing is to check whether the denominators are the same and if not can we do to fix that. Notice that in this case we don't need to change the second fraction because 3 is a factor of 6. What we would do instead is change the first fraction to have 6 as the denominator by multiplying by $\frac{2}{2}$.

$$\frac{1 \times 2}{3 \times 2} + \frac{1}{6} = \frac{2}{6} + \frac{1}{6} = \frac{3}{6}$$

From here we can see that the fraction can be simplified further. A factor of 3 can be taken out of the top and bottom leaving us with:

$$\frac{3 \times 1}{3 \times 2} = \frac{\cancel{3} \times 1}{\cancel{3} \times 2} = \frac{1}{2}$$

Example: Express $\dfrac{1}{x+1} - \dfrac{1}{x-1}$ as a single fraction.

Solution: To do this we will multiply the denominators to get $(x+1)(x-1)$ as the new denominator.

$$\left(\frac{1}{x+1} \times \frac{x-1}{x-1}\right) - \left(\frac{1}{x-1} \times \frac{x+1}{x+1}\right)$$

$$= \frac{x-1}{(x+1)(x-1)} - \frac{x+1}{(x+1)(x-1)} = \frac{(x-1)-(x+1)}{(x+1)(x-1)} = \frac{-2}{(x+1)(x-1)}$$

Being able to work with fractions is good as you don't always need a calculator to calculate them unlike if you exclusively used decimals for all calculation.

1.4 Percentages

Percentages express how large one quantity is relative to another quantity; so for example percentage yields express how large the yield of a reaction is compared to the theoretical yield. A percentage of a quantity is a way of expressing a number as a fraction of 100. The symbol for percentage is %.

In general if we have quantities x and y and we want to express how large x is compared to y (i.e. what percentage is x of y?) we can use the formula:

$$\boxed{\text{percentage} = \frac{x}{y} \times 100\%}$$

Example: What percentage is 8 of 160?

Solution:

$$\frac{8}{160} \times 100\% = 5\%$$

We may also want to calculate the percentage of a quantity for example, what is 28% of 132? In general we can use the formula:

$$\boxed{x = \frac{\text{percentage}}{100\%} \times y}$$

Example: What is 28% of 132?

Solution:

$$x = \frac{28\%}{100\%} \times 132 = 36.96$$

Chemistry Example: In the esterification reaction

$$CH_3OH + CH_3COOH \longrightarrow CH_3COOCH_3 + H_2O$$

the reactants combine in the following proportions based on their molar masses: 32g of CH_3OH reacts with 60g of CH_3COOH to form 74g of the ester product.

In a particular reaction 1.8g of methanol is mixed with an excess of ethanoic acid. At the end of the experiment 2.6g of the ester is extracted. What is the percentage yield?

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical maximum yield}} \times 100\%.$$

Solution: First we need to calculate the theoretical maximum yield:

From the question we know that 32g of CH_3OH yields 74g of ester.

Dividing through by 32 gives us that 1g of CH_3OH yields $\frac{74}{32}$g of ester.

Multiplying by 1.8 gives us that 1.8g of CH_3OH yields $1.8 \times \frac{74}{32} = 4.2$g of ester.

We know from the question the actual yield is 2.6g so using the percentage yield formula we have

$$\text{percentage yield} = \frac{2.6\text{g}}{4.2\text{g}} \times 100\% = 61.9\%.$$

Note: We may wish to convert between fractions and percentages:

1. To convert a fraction to a percentage we multiply the fraction by 100%. For example, $\frac{1}{2}$ as a percentage is $\frac{1}{2} \times 100\% = 50\%$.

2. To convert a percentage to a fraction we divide the percentage by 100% and simplify. For example, 25% as a fraction is $\frac{25\%}{100\%} = \frac{1}{4}$.

1.5 Rounding, Significant Figures and Decimal places

Rounding

We round numbers as follows:

1. Decide to which 'nearest' number or decimal point to round to.
2. Leave it the same if the next digit is less than 5 (rounding down).
3. Increase it by 1 if the next digit is 5 or more (rounding up).

Example: Round 467 to the nearest 10.

Solution: So the answer is 470 (we round up to 470 as the digit after the 6 is a 7).

Example: Round 0.314 to 2 decimal places.

Solution: So the answer is 0.31 (we round down to 0.31 as the digit after the 1 is a 4).

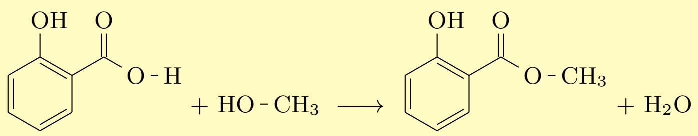
Significant Figures

Significant figures are used to give us an answer to the appropriate precision. We use s.f. as a short hand for significant figures. So we write a number to a given number of significant figures as follows:

- When asked to write a number to n significant figures we only display the first n non-zero digits.
- Therefore an answer may require rounding up or down. For example, a temperature of 37.678°C to 3 s.f. is 37.7°C.
- For positive decimals less than 1 we start counting the number of significant figures from the first non-zero number. For example, 0.009436 to 2 s.f. is 0.0094 and not 0.00.
- We use significant figures on negative numbers in the same way. For example, -137.54 to 2 s.f. is -140.

IMPORTANT: When multiplying or dividing numbers expressed to different numbers of significant figures we leave our answer to smallest number of significant figures used in the numbers we have multiplied or divided.

Chemistry Example: Below we have the reaction of methanol and salicylic acid to from the ester methyl salicylate.



The rate of formation of the ester is given by the expression:

$$\text{rate} = k[\text{methanol}][\text{salicylic acid}]$$

where k is the rate constant. What is the rate when $k = 3.057\ (\text{mol dm}^{-3})^{-1}\text{s}^{-1}$, $[\text{methanol}] = 3\ \text{mol dm}^{-3}$ and $[\text{salicylic acid}] = 0.86\ \text{mol dm}^{-3}$?

Solution: So substituting these values into the rate equation gives:

$$\text{rate} = 3.057 \times 3 \times 0.86 = 7.88706\ \text{mol dm}^{-3}\text{s}^{-1}$$

Now our concentration of methanol was expressed in the fewest number of significant figures, in fact to 1 s.f. so we should also leave our answer to 1 s.f.

$$\text{rate} = 8\ \text{mol dm}^{-3}\text{s}^{-1}$$

Decimal Places

The correct number of decimal places is used to indicate the correct precision when adding or subtracting. Consider the number 4.5312 which is given to 4 d.p. (decimal places). However we could also write this number to 1 d.p. which would be 4.5.

Example: A Baker is making a cake and adds to the mixture 100.0g of flour, 40.2g of sugar and 50.134g of eggs. Calculate the total mass of the cake to the correct number of decimal places.

Solution: The issue is that the masses in the question are given to different numbers of decimal places. So we must follow these steps:

1. Add or subtract as normal including all the decimal places.
2. Round the answer to the smallest number of decimal places of the items used in step 1.

Applying these rules to the example:

1. $100.0\text{g} + 40.2\text{g} + 50.134\text{g} = 190.334\text{g}$
2. Now the smallest number of decimal places in the items we summed in step 1. is 1 d.p. from the 100.0g of flour and 40.2g of sugar so we round our answer from part 1 to 1 d.p. to get the answer 190.3g.

1.6 Equations and Functions

Physical and chemical quantities are often linked in equations.

variables

$$y = ax + b$$

coefficient of x constants

- Variables are quantities that can take different values; they can vary.
- Constants are fixed numbers so unlike variables cannot change.
- The coefficient of x is the constant before the x. In the same way for the equation $y = 8t^2 + t$ the coefficient of t^2 is 8 and the coefficient of t is 1.

What is a Function?

Relationships between quantities are referred to as functions which we usually denote $f(x)$, pronounced 'f of x'.

In general we have y is a function of x:

$$y = f(x)$$

This means that y is equal to an expression 'made up' of x's. For example $y = x + 3$ or $y = e^{3x}$.

- So a function takes a quantity (a variable or number) and applies operations to it. This produces new quantity.
- Although we have used the notation $f(x)$ there is no reason why we could not use $g(x)$ or even $\phi(x)$.
- We can also have $f(z)$ or $g(\theta)$ if we have functions 'made up' of variables other than x. For example $f(z) = z^2$ and $g(\theta) = \cos(\theta)$.

Note: We can often think of $f(x)$ and y as interchangeable.

Example: The function f takes a variable, doubles it and then subracts 2. The function g halves its input. What is:

1. $f(3)$?
2. $f(x)$?
3. $g(8)$?

Solution:

1. The function f takes the input and doubles it then subtracts 2. With the input being 3, we can find $f(3)$ by applying those steps to the number 3. When we double it we get 6. Subtract 2 then gives us 4. So our final answer is $f(3) = 4$.
2. We do these same steps but with the variable x instead of a number. First we double it to give $2x$. Then we subract 2 to give $2x - 2$. We now have that $f(x) = 2x - 2$.
3. We apply the function g to 8. Halving 8 will give us 4, hence $g(8) = 4$.

Chemistry Example: In an experiment, the pressure of a gas is monitored as the temperature is changed, while the volume and amount of gas remain constant and the following relationship was established:

$$p = 0.034T$$

1. Identify the variables and coefficients in the equation.

2. What is p a function of?

3. Given that $T = 343$ what is the value of p?

Solution:

1. In the experiment, p can vary and T can also vary. This means that p and T are both **variables**. The 0.034 is multiplying the T, making it a coefficient. The coefficient of p is 1.

2. In the equation $p = 0.0341T$ the only other variable apart from p is T. Hence p is a function of T and T alone.

3. To find this we will substitute 343 for T into the equation to get, $p = 0.0341 \times 343 = 11.662 = 11.7$ (to 3 s.f.)

Functions with Multiple Variables

Functions can also be of multiple variables. The function:

$$y = f(x, z)$$

means that the function f takes in a value of x and also a value of z to give an output so x and z are both variables. For example:

$$y = f(x, z) = xz + 2x + 2$$

This function would input variables x and z and give their product plus $2x$ plus 2 as an output. If $x = 2$ and $z = \frac{1}{2}$ then $y = 7$.

Chemistry Example:

Consider the ideal gas equation:

$$pV = nRT.$$

The temperature T can be expressed as a function of pressure p and volume V which are variables. This can be written as:

$$T = f(p, V) = \frac{pV}{nR}$$

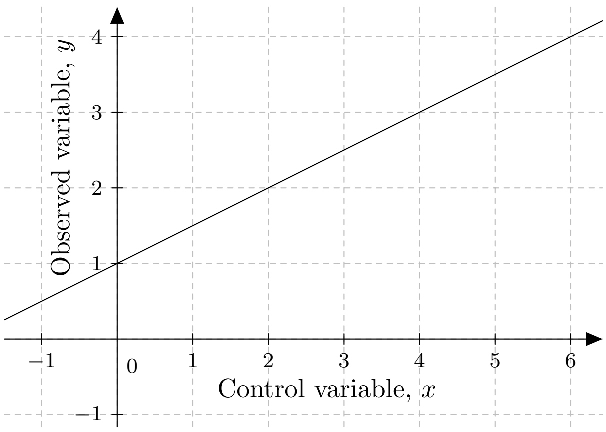
Note: You wouldn't say that T is a function of n and R since they are constants and not variables and therefore T does not depend on them.

1.7 Graphs

Plotting data on a graph has the major advantage it is often clear to see trends and patterns that are present. In experiments we have:

- a control variable that we can change,
- an observed variable that we measure,
- and all other quantities we try and keep constant.

When plotting a graph of data we always plot the control variable along the horizontal (or x) axis and the observed variable along the vertical (or y) axis.



Straight Line Graphs

Straight line graphs come in the form:

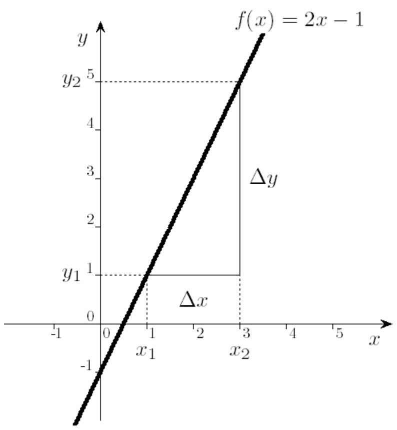
$$\boxed{y = mx + c}$$

where x is the controlled variable, y is the observed variable and m and c are constants.

- c is known as the intercept and is where the graph passes through the y-axis. Hence to find c we find the value of y when $x = 0$.
- m is known as the gradient and describes how steep the line is. It can be found by drawing a 'triangle ' on the straight line and using it to calculate the equation:

$$m = \frac{\Delta y}{\Delta x}$$

This can all be visualised on the graph below:



When x increases from 1 to 3 we have that y increases from 1 to 5. Hence

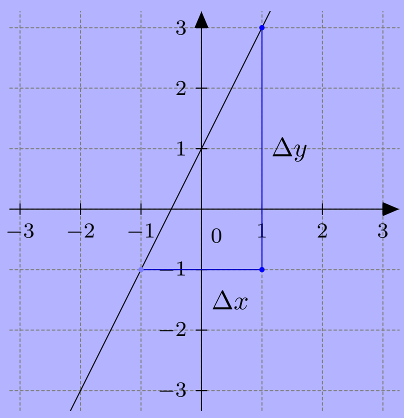
$$\Delta x = 3 - 1 = 2$$

$$\Delta y = 5 - 1 = 4$$

So the gradient $m = \dfrac{\Delta y}{\Delta x} = \dfrac{4}{2} = 2$

The intercept c is where the graph passes through the y-axis hence from the graph we can see $c = -1$.

Example: What is the equation of the straight line shown in the diagram below?



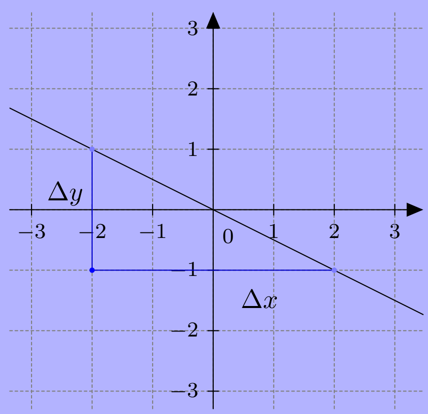
Solution: We know that since this a straight line it will be in the form $y = mx + c$. The value of c is the value of y when $x = 0$. At $x = 0$, $y = 1$ from the graph. Therefore $c = 1$.

To find m we need to calculate $\dfrac{\Delta y}{\Delta x}$. Using the triangle method with the triangle in the above graph gives:

$$\text{gradient} = \frac{\Delta y}{\Delta x} = \frac{y_2 - y_1}{x_2 - x_1} = \frac{3 - (-1)}{1 - (-1)} = \frac{4}{2} = 2$$

Since $m = 2$, the equation of the line is $y = 2x + 1$.

Example: What is the equation of the straight line shown in the diagram below?



Solution: Since this a straight line it will be in the form $y = mx + c$. The value of c can be seen to be 0, because when $x = 0$, y is also 0.

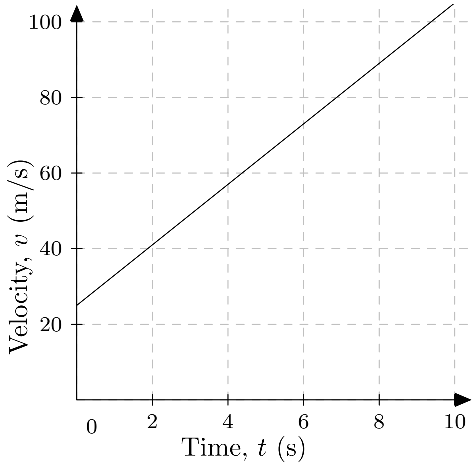
Using the triangle method we can find the gradient of the line. With the triangles on the graph we have:

$$\text{gradient} = \frac{\Delta y}{\Delta x} = \frac{y_2 - y_1}{x_2 - x_1} = \frac{-1 - 1}{2 - (-2)} = \frac{-2}{4} = -\frac{1}{2}$$

Combining this altogether gives us that the equation of this line is, $y = -\dfrac{1}{2}x$.

Graphs with Units

Often graphs won't be those of just numbers and a line but instead will have some physical significance and hence include units. Consider the graph of a particle's velocity as a function of time:



The equation of the line is $v = 8t + 25$. v has units of metres per seconds and to make the equation work so everything on the right hand side must also have units of metres per second as well. That means that the $c = 25$ has units of m/s. This 25 m/s is the starting velocity of the particle.

The units of m can be worked out from the equation:

$$\frac{\Delta y}{\Delta x} \text{ or in this case } \frac{\Delta v}{\Delta t}$$

Δv has the same units as v (m/s) and similarly Δt has the units (s). This means m, the gradient, has units of m/s $\div$ s or m/s^2. Since the gradient has units of distance per time squared, then it means that it is an acceleration. The particle will accelerate at 8m/s^2.

2 Algebra

2.1 Powers

Powers are a way to write that we have multiplied a number by itself a given number of times. For example 4 squared is $4^2 = 4 \times 4$ and 5 cubed would be $5^3 = 5 \times 5 \times 5$. So more generally, for any positive whole number n:

$$\boxed{x^n = \underbrace{x \times x \times \ldots \times x}_{n \text{ times}}}$$

- We call x the **base**.
- We call n the **index of the base** or its **power**.

We would either say x^n as 'x raised to the power of n', 'x to the power of n' or 'x to the n'.

Example:

So we can write $T \times T \times T \times T \times T$ as T^5. (Note that T is the base and the power is 5).

Example:

It is worth noting when a negative number is raised to an even power then the answer is positive.

$$(-2)^4 = -2 \times -2 \times -2 \times -2 = 16$$

Negative Powers

We can also have negative numbers as powers, these give fractions called reciprocals for example $2^{-1} = \frac{1}{2}$. So more generally:

$$\boxed{\begin{array}{c} x^{-n} = \dfrac{1}{x^n} \\ \text{As long as } x \neq 0 \end{array}}$$

Example:

So we can write $\dfrac{1}{qqqqqq}$ as $\dfrac{1}{q^6}$ which is q^{-6}.

We can simplify multiple terms like in the examples below by collecting together the terms which are the same.

Example:

So we can simplify $cccdcd$ to c^4d^2. (Note that we have collected all the c and d together separately).

Example:

So we can simplify $\dfrac{xxyzzzz}{abbb}$ to $\dfrac{x^2yz^4}{ab^3}$ which we can then write as $x^2yz^4a^{-1}b^{-3}$.

Special Cases

1. Any non zero number raised to the power of 1 is itself, for example $3^1 = 3$ and $15^1 = 15$. So we have:

$$\boxed{x^1 = x}$$

Note: Usually we do not write bases to the index of 1 we just write the base. So we would write x and not x^1.

2. If a number is rasied to the power of 0 then the answer is 1. For example $4^0 = 1$ and $(-454.786)^0 = 1$. So we have:

$$\boxed{x^0 = 1}$$

Rules for Powers

We have the following three rules for when working with powers:

1. $x^a \times x^b = x^{a+b}$
2. $\dfrac{x^a}{x^b} = x^{a-b}$
3. $(x^a)^b = x^{a \times b}$

Example:

So we can simplify $\dfrac{y^3z^2y^4}{z^6}$ to $y^{3+4}z^{2-6}$ which is y^7z^{-4} (we have used rules 1 and 2 here).

Example:

So we can simplify $(a^3b^2ca)^2$ using rule 1 to $(a^{3+1}b^2c)^2$ to $(a^4)^2(b^2)^2(c)^2$ which we can then write by using rule 3 as $a^8b^4c^2$.

Roots

The opposite of squaring a number say $4^2 = 16$ is finding the square root in this case $\sqrt{16} = 4$. Note the notation for square root is $\sqrt{\ }$. The same is true for cubing and cube roots which are denoted $\sqrt[3]{\ }$. For example $3 \times 3 \times 3 = 27$ so $\sqrt[3]{27} = 3$. In general the opposite of raising a number x to the power of n is to find the n^{th} root which is denoted $\sqrt[n]{\ }$.

We also use fractional powers as another, often more useful way, to write roots. So we have that $\sqrt{x} = x^{\frac{1}{2}}$ and $\sqrt[3]{x} = x^{\frac{1}{3}}$. More generally we have:

$$\boxed{x^{\frac{1}{n}} = \sqrt[n]{x}}$$

Note: A root written in its fractional form is often must easier to manipulate with the algebraic rules for powers.

Example:

A numerical example: since $\sqrt[5]{32} = 2$ we could also write $32^{\frac{1}{5}} = 2$.

Example:

So we can write $\dfrac{\sqrt{x}}{x} = \dfrac{x^{\frac{1}{2}}}{x} = x^{\frac{1}{2}-1} = x^{-\frac{1}{2}}$.

Example: Simplify the following: $\dfrac{\sqrt[3]{ab^3}(ac^4)^2}{a^{\frac{4}{3}}b}$

The first thing that we can do is expand the brackets on the numerator to give:

$$\begin{aligned}
\frac{\sqrt[3]{ab^3}(ac^4)^2}{a^{\frac{4}{3}}b} &= \frac{\sqrt[3]{ab^3}a^2c^8}{a^{\frac{4}{3}}b} && \text{The cube root can now be simplified}\\
&= \frac{a^{\frac{1}{3}}ba^2c^8}{a^{\frac{4}{3}}b} && \text{All the powers can be collected}\\
&= a^{\frac{1}{3}-\frac{4}{3}+2}\ b^{1-1}\ c^8 && \text{This can be simplified}\\
&= a^{-1+2}\ b^0\ c^8\\
&= ac^8
\end{aligned}$$

2.2 Rearranging Equations

Rearranging equations is changing the arrangement of terms in an equation. Consider the ideal gas equation $pV = nRT$. We could rearrange the equation so that we have T in terms of the other variables, so in this case $T = \frac{pV}{nR}$. This rearranging is called making T the subject of the formula. When rearranging we perform operations to both sides of the equation so we may:

- Add or subtract the same quantity to or from both sides.
- Multiply or divide both sides by the same quantity.

Order to do Rearrangements

BODMAS is used to decide which operations we should undo to make our quantity the subject. It is used in reverse, so the operations are undone in the following order:

1. Subtraction
2. Addition
3. Multiplication
4. Division
5. Orders
6. Brackets

Note: As we mentioned in Section 1.1, addition and subtraction have the same priority so can be done in either order. The same is true for multiplication and division.

Chemistry Example: An ion is moving through a magnetic field. After a time t the ion's velocity has increased from u to v. The acceleration is a and is described by the equation $v = u + at$. Rearrange the equation to make a the subject.

Click here for a video example

Solution: We identify the operations in use are $+$ and $\times$. Then we undo (or invert) each of the operations. Remember that we can do anything as long as we do it on both sides of the $=$ sign.

$$v = u + at$$

We start by undoing the addition as we go in the order of BODMAS backwards. On the right hand side we have u being added to the term involving a. We then invert the operation by doing the opposite and subtracting u from both sides of the equation. So

$$v = u + at$$
$$\implies v - u = u - u + at$$
$$\implies v - u = at$$

We can now see that the only other operation acting on our a is multiplication which we undo by dividing both sides of the equation by t:

$$\implies \frac{v-u}{t} = \frac{at}{t}$$
$$\implies \frac{v-u}{t} = \frac{a\cancel{t}}{\cancel{t}}$$
$$\implies a = \frac{v-u}{t}$$

We now have made a the subject of this equation.

Chemistry Example: In thermodynamics, the Gibbs Function ΔG dictates whether a reaction is feasible at a temperature T. ΔS and ΔH are the entropy and enthalpy changes for the reaction. They are all related by the following equation:

$$\Delta G = \Delta H - T\Delta S$$

Rearrange this equation to make ΔS the subject.

Solution: The first step is to undo the subtraction on the right hand side by adding $T\Delta S$ to each side. This produces the equation:

$$\Delta G + T\Delta S = \Delta H$$

The next step would be to undo the addition by subtracting ΔG from both sides to get the term involving ΔS on its own. Doing this step gives:

$$T\Delta S = \Delta H - \Delta G$$

This leaves only the multiplication to be dealt with, which is undone by dividing by T to give the equation for ΔS to be:

$$\Delta S = \frac{\Delta H - \Delta G}{T}$$

Rearranging with Powers and Roots

The inverse operations of powers are roots, so to reverse a power we take a root and vice versa. We complete rearrangement in reverse order of BODMAS therefore we rearrange powers and roots in the orders section.

Example: Einstein's equation for mass energy equivalence is often seen in the form:

$$E = mc^2$$

Express it with c being the subject.

Solution: To start with we would divide each side of the equation by m.

$$\frac{E}{m} = \frac{mc^2}{m} \implies \frac{E}{m} = \frac{\cancel{m}c^2}{\cancel{m}} \implies \frac{E}{m} = c^2$$

Now c is raised to the power of 2. To undo this operation we take the square root of both sides.

$$\frac{E}{m} = c^2 \implies \sqrt{\frac{E}{m}} = \sqrt{c^2} \implies \sqrt{\frac{E}{m}} = c$$

Note: If we were to make a the subject in the equation $a^2 = b + c$ we take the square root of the whole of both sides of the equation to get $a = \sqrt{b+c}$ and **not** $a = \sqrt{b} + \sqrt{c}$.

Note: Similarly if we were to make d the subject in the equation $\sqrt{d} = e + f$ we square the whole of both sides of the equation to get $d = (e+f)^2$ and **not** $d = e^2 + f^2$.

Example: Solve the following:

1. Given $px + a = qx + b$ make x the subject of the formula.
2. Given $\frac{\sqrt{t}+2}{y} = y$ make t the subject of the equation.
3. Make P the subject of the equation $x(1+P)^2 = \frac{4}{x}$

Click for video example of Question 3

Solution:

1. We have an x on both sides of the equation $px + a = qx + b$ so we need to collect these together, first by subtracting qx from both sides to get:

$$
\begin{aligned}
px + a - qx = qx + b - qx & \quad \text{Then factorise and simplify} \\
x(p-q) + a = b & \quad \text{Subtract } a \text{ from both sides} \\
x(p-q) + a - a = b - a & \quad \text{Now simplify} \\
x(p-q) = b - a & \quad \text{Divide both sides by } (p-q) \\
x = \frac{b-a}{p-q} & \quad \text{Hence } x \text{ is now the subject}
\end{aligned}
$$

2. We notice that the only t is on the top of the fraction and underneath a square root. The first step would be to multiply both sides by y to get:

$$
\begin{aligned}
\sqrt{t} + 2 = y^2 & \quad \text{Take away 2 from both sides} \\
\sqrt{t} = y^2 - 2 & \quad \text{Square both sides to remove the root} \\
t = (y^2 - 2)^2 & \quad \text{Hence } t \text{ is now the subject}
\end{aligned}
$$

3. The P is inside a bracket which is being squared and multiplied. The first step would be to divide both sides by x to give:

$$
\begin{aligned}
(1+P)^2 = \frac{4}{x^2} & \quad \text{Take the square root of both sides} \\
1 + P = \sqrt{\frac{4}{x^2}} & \quad \text{This square root can be simplified down, since the numerator} \\
& \quad \text{and denominator are both squares} \\
1 + P = \frac{2}{x} & \quad \text{Subtract 1 from both sides} \\
P = \frac{2}{x} - 1 & \quad \text{Hence } P \text{ is now the subject}
\end{aligned}
$$

Click here for a video example on a similar question

2.3 Physical quantities, Units and Conversions

Often we don't just have numbers on their own, they are connected to physical quantities that can be measured such as time, concentration, mass or velocity. When describing a quantity, units are needed to define what it means physically. There is a lot of difference between 200 degrees Celsius, 200 Kelvin and 200 degrees as an angle!

All quantities share the same format:

$$\boxed{\text{Variable} = \text{Number} \times \text{Units}}$$

E.g. suppose we have the mass m of the product is $m = 1.2\,\text{g}$. Then the mass m is the variable, 1.2 is the number and g grams are the units.

- Any terms in an equation that are added or subtracted need to have the same units in order to produce an answer that makes sense. For example the sum 3kg + 12s doesn't make physical sense.
- However different units can be multiplied together and divided to make a new compound unit.

Example: Speed is calculated from the equation:

$$\text{Speed} = \frac{\text{Distance}}{\text{Time}}$$

Distance is measured in metres m and time is measured in seconds s. What are the units of speed?
Solution: To do this we replace the terms in the equation with their units.

$$\text{Units of Speed} = \frac{\text{m}}{\text{s}}$$

This means that this speed is measured in metres per second $\frac{\text{m}}{\text{s}}$. This can also be denoted by m/s or ms^{-1}.

Note: If a unit has a negative power then it is said to be per that unit. For example kJ mol^{-1} is pronounced as kilo-joules **per** mole.

Base Units

There are 7 fundamental quantities in all of science which all other quantities are built from. These with their SI units are:

- Length measured in meters m.
- Mass measured in kilograms kg.
- Time measured in seconds s.
- Temperature measured in kelvin K.
- Amount of substance measured in moles mol.
- Electric current measured in amperes A.
- Luminous intensity measured in candelas cd.

The main ones we are interested in for chemistry are mass, time, temperature, amount of substance and length. From these we can construct a whole host of other units such as newtons N and pascals Pa.

Chemistry Example: Find the units of the molar gas constant R using the ideal gas equation $pV = nRT$ where p is measured in kg m^{-1} s^{-2}, V in m^3, n in mol and T in K.

Solution: To begin we should rearrange the equation to make R the subject as it's easier to do this before putting the units in. So divide both sides of the equation by nT to give:

$$\frac{pV}{nT} = \frac{nRT}{nT} \Longrightarrow \frac{pV}{nT} = R$$

Now we can substitute the units into this equation and then group the powers.

$$\text{Units of } R = \frac{\text{kg m}^{-1}\text{s}^{-2}\text{m}^3}{\text{mol K}} = \frac{\text{kg m}^2\text{s}^{-2}}{\text{mol K}} = \text{kg m}^2\text{s}^{-2}\text{mol}^{-1}\text{K}^{-1}$$

It might look ugly but many physical constants have complex units.

Note: Calculating units is a good way of checking an equation has been manipulated correctly since the units must be equal on both sides. For example if the left hand side of the equation has units of mass per temperature then the right hand side must do as well.

Unit prefixes and Scientific Notation

The numbers used in chemistry range dramatically from being very large like Avogadro's number to incredibly small such as Planck's constant so we use either prefixes or scientific notation to display numbers in a concise form. Take the kilogram for example, it means 1000 grams because it uses the prefix kilo k to mean $\times 10^3$ (which is 1000).

The SI prefixes that you are expected to know are shown in this table below.

Prefix	Symbol	Power of 10
Atto	a	10^{-18}
Femto	f	10^{-15}
Pico	p	10^{-12}
Nano	n	10^{-9}
Micro	μ	10^{-6}
Milli	m	10^{-3}
Centi	c	10^{-2}
Deci	d	10^{-1}
1	**1**	$\mathbf{10^0}$
Kilo	k	10^3
Mega	M	10^6
Giga	G	10^9
Tera	T	10^{12}
Peta	P	10^{15}

Example: Express the world's population using an SI prefix to 1 significant figure.

Solution: At time of writing the world's population is 7 billion people to 1 significant figure or 7,000,000,000. This can be written as $7 \times 1,000,000,000 = 7 \times 10^9$. 10^9 has to prefix Giga, G, so the population would be 7 Giga-people.

Scientific notation (or standard form) is another way of writing incredibly large or small numbers. Instead of writing the number to the nearest SI prefix, we write the number as one (non-zero) digit followed by the decimal places all multiplied by the appropriate power of ten. For example 3112 is 3.112×10^3 in standard form.

Chemistry Example: Avogadro's constant N_a is 602 200 000 000 000 000 000 000 to 4 significant figures. Express it in standard form.

Solution: We need to first find the nearest power of 10. To do this we count how many places are after the first digit. There are 23 places after the (first digit), so the power of 10 will be 23, 10^{23}.

The appropriate decimal number would be 6.022, since that has a single digit followed by the decimal places.

This then makes Avogadro's constant 6.022×10^{23} to 4 s.f.

Converting between Units

For some measurements chemists prefer to use non-SI units because they produce nicer numbers to work with. For example the Ångström (Å) is a unit of length with 1Å$= 10^{-10}$m hence is more appropriate unit when working with atomic spacings.

IMPORTANT: When substituting numerical values into equations to find another quantity we must substitute the values in their SI form. For example when working in Ångström's we would first have to convert our answer to metres before substituting.

Example: The temperature outside is measured to be 95°F. Given that Fahrenheit and Celsius are linked by the equation:

$$\mathrm{C} = \frac{5}{9} \times (\mathrm{F} - 32)$$

and Celsius and Kelvin are linked by the equation:

$$\mathrm{K} = \mathrm{C} + 273$$

Calculate the outside temperature in Kelvin.

Solution: We need to apply 2 changes in units, first from F to C and then from C to K. We know the the temperature is 95°F. Hence using the equation below we can find the temperature in Celsius:

$$\mathrm{C} = \frac{5}{9} \times (\mathrm{F} - 32) = \frac{5}{9} \times (95 - 32) = \frac{5}{9} \times 63 = 35.$$

The temperature in Celsius is 35°. Now all that is needed to do is put this into the equation below to find the temperature in Kelvin:

$$\mathrm{K} = \mathrm{C} + 273 = 35 + 273 = 308.$$

Chemistry Example: An industrial chemist produces 2.5×10^5 dm^3 of fertiliser in a reaction. How much is that in m^3?

Solution: First we need to find how many m^3 there are per dm^3. So we start with 1m^3.

$$1\mathrm{m}^3 = (1\mathrm{m})^3$$

We know what the conversion between m and dm from our prefixes table is 1dm = 0.1m which means that 1m = 10dm. Substituting this back in gives:

$$\begin{aligned} (1\mathrm{m})^3 &= (10\mathrm{dm})^3 && \text{Expand this out} \\ 1\mathrm{m}^3 &= 10^3\mathrm{dm}^3 && \text{Divide through by } 10^3 \\ 10^{-3}\mathrm{m}^3 &= 1\mathrm{dm}^3 \end{aligned}$$

We have a relation that allows us to put in dm^3 and get out what it is in m^3.

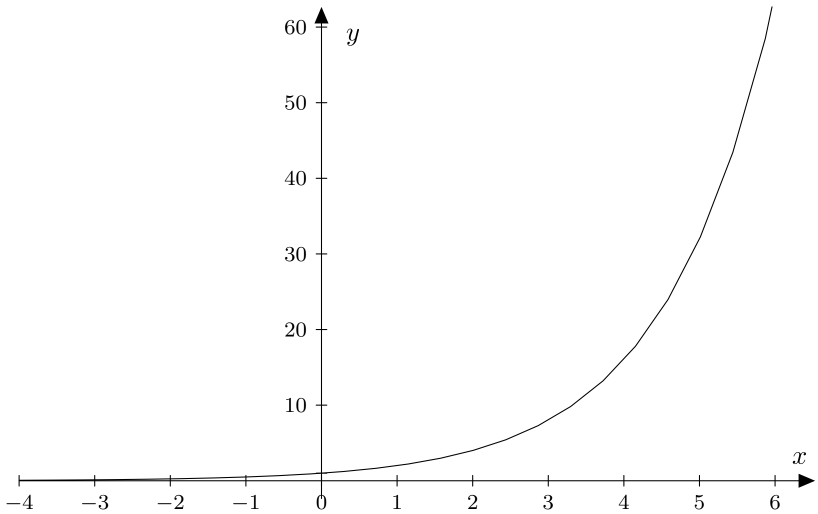
$$2.5 \times 10^5 \ \mathrm{dm}^3 = 2.5 \times 10^5 \times 10^{-3} \ \mathrm{m}^3$$
$$\implies 2.5 \times 10^5 \ \mathrm{dm}^3 = 2.5 \times 10^2 \ \mathrm{m}^3$$

2.4 Exponentials

We may use the term 'exponential growth' as a way to describe the rate of a reaction as the temperature increases. In using this phrase we are describing a very fast rate of increase. We can represent this idea mathematically with one of the simplest exponential equations:

$$\boxed{y = a^x}$$

where a is a constant, x is the controlled variable (in the above case temperature) and y is the observed variable (in the above case rate of reaction).



Above we have the graph of $y = 2^x$ and we can see the graph increases at very fast rate which is what we would expect with exponential growth. Other mathematical things to note are:

- The graph passes through the point $(0, 1)$ as any variable raised to the power of 0 is equal to 1.
- The values of y are small and positive when x is negative.
- The values of y are large and positive when x is positive.

The Exponential Function

So far we have used the word exponential to describe equations in the form $y = a^x$ however the word is usually reserved to describe a special type of function. It is quite likely we will have seen the symbol π before and know it represents the infinite number $3.14159265\ldots$ In this section we will be working with the number:

$$e = 2.7182818\ldots$$

Like π, e is another number that goes on forever! When we refer to ***the*** exponential function we mean $y = e^x$. This can be seen as a special case of the previous section when the constant is $a = e$ in the equation $y = a^x$. When we refer to e^x we say 'e to the x'.

Note: Another notation for e^x is $\exp(x)$. They mean the same thing.

Chemistry Example: The Arrhenius equation below describes the exponential relationship between the rate of a reaction k and the temperature T

$$k = A\exp\left(-\frac{E_a}{RT}\right)$$

where R, E_a and A are all constants. Suppose for a reaction that the activation energy is $E_a = 52.0$ kJ mol^{-1}, the gas constant $R = 8.31$ J K^{-1} mol^{-1} and $A = 1.00$. What is the rate of the reaction k when the temperature $T = 241$ K?

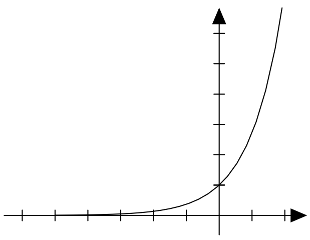
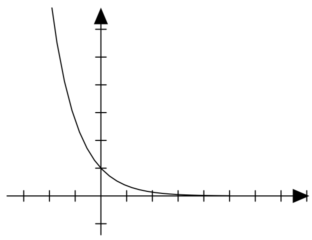
Solution: We substitute our given values from the question into the Arrhenius equation.

$$k = A\exp\left(-\frac{E_a}{RT}\right) = 1 \times \exp\left(-\frac{52 \times 10^3}{8.31 \times 241}\right)$$
$$\Longrightarrow k = \exp(-25.9648\dots)$$
$$\Longrightarrow k = 5.2920\dots \times 10^{-12}$$
$$\Longrightarrow k = 5.29 \times 10^{-12} \text{ (to 3 s.f.)}$$

Remember we can use the e button on our calculator to find the final answer.

Exponential Graphs

Exponential graphs follow two general shapes called growth and decay which are shown below.

- On the left exponential growth which is represented by the equation $y = e^x$ note that the graph gets steeper from left to right.
- On the right exponential decay which is represented by the equation $y = e^{-x}$ note that the graph gets shallower from left to right.

Algebraic Rules for Exponentials

We use very similar rules as the ones we had for powers. The only difference is that the base in now a constant and the power is a variable.

1. $a^x \times a^y = a^{x+y}$
2. $\dfrac{a^x}{a^y} = a^{x-y}$
3. $(a^x)^y = a^{x\times y}$

Note: Above we have that x and y are variables and a is a constant for example $a = e$ or $a = 3$. And in order to use the rules a must be the same for all terms. For example we can not simplify $e^x \times 3^x \times 4^x$.

Example: Simplify the following equations:

1. $y = 3^x \times 3^{2x}$
2. $y = \dfrac{2^x}{4}$
3. $y = \left(e^{-x+1}\right)^x$

Solution:

1. Since the bases are the same we use the first rule.
$$y = 3^x \times 3^{2x} = 3^{x+2x} = 3^{3x}$$
2. The first thing we notice is that 4 can be written as 2^2 so:
$$y = \frac{2^x}{2^2}.$$
Now are we have powers to the same base we can apply the rules. Using the second rule we have:
$$y = 2^{x-2}$$
3. Using the third rule we get that:
$$y = e^{(-x+1)\times x} = e^{-x^2+x}$$

2.5 Logarithms

Just as addition and multiplication have inverses (subtraction and division) so we have inverses for exponentials. These are called logarithms. A logarithm answers the question 'how many of one number do we multiply to get another number?'

Example: How many 2's do we multiply to get 8?

Solution: $2 \times 2 \times 2 = 8$ so we need to multiply 3 of the 2's to get 8. So the logarithm is 3.

We have a notation for logarithms for example the last example would be written as:

$$\log_2(8) = 3$$

where this tells us we need multiply 2 by itself 3 times to get 8.

So more generally we can write:

$$\boxed{\log_a(x) = y}$$

- This tells us we need multiply a by itself y times to get x. (In other words $x = a^y$).
- We say that a is the base of the logarithm.

We can see clearly that as logarithms are the inverse of exponents there exists a relationship between the two given by:

$$\boxed{\text{If } y = a^x \text{ then } x = \log_a(y)}$$

Example: Write $81^{0.5} = 9$ as a logarithm.

Solution: So we need to multiply 81 by itself 0.5 times to get 9 so we have $\log_{81}(9) = 0.5$

Example: If $10^x = 3$ then find x.

Solution: We need to multiply 10 by itself x times to get 3 so we have:

$$x = \log_{10}(3) = 0.477 \text{ to 3 s.f.}$$

Logarithms are useful for expressing quantities that span several orders of magnitude. For example the pH equation $\text{pH} = -\log_{10}[\text{H}^+]$ as small change in pH results in a very large change in $[\text{H}^+]$.

Logarithms: The Inverses of Exponentials

As taking a logarithm is the inverse of an exponentials to the same base. We can cancel them using the rules below.

$$\boxed{\log_a(a^x) = x}$$

$$\boxed{a^{\log_a(x)} = x}$$

IMPORTANT:

1. When cancelling in the first case all the quantities in the logarithm must be contained in the 'power' of the exponential. For example $\log_a(a^x + 3) \neq x + 3$ as the 3 is not part of the power of the exponential.

2. When cancelling in the second case all of the power must be contained in the logarithm. For example $a^{\log_a(x)+4} \neq x + 4$ as the 4 is not in the logarithm.

Example: Simplify the following:

1. $\log_{10}(10^{5x^3+3x})$
2. $3^{\log_3(x^7+1)}$
3. $\log_3(10^{4x})$
4. $a^{\log_a(4x^3)+2x}$
5. $\log_8(8^{2x^4}+7)$

Solution:

1. $\log_{10}(10^{5x^3+3x}) = 5x^3+3x$
2. $3^{\log_3(x^7+1)} = x^7+1$
3. We cannot simplify this as the logarithm has the base 3 and the exponential is to the base 10.
4. First note that $a^{\log_a(4x^3)+2x} \neq 4x^3+2x$. We do this as follows:
$$a^{\log_a(4x^3)+2x} = a^{\log_a(4x^3)}a^{2x} = 4x^3a^{2x}$$
5. We cannot simplify in this case as the 7 is not part of the exponential.

Logarithms to the Base 10

Many equations in chemistry include logarithms and we tend to use only two logarithms to different bases. The first one is to the base 10 such as in the pH equation $\text{pH} = -\log_{10}[\text{H}^+]$. In the usual notation we would write $\log_{10}$ however we tend to write logs to the base 10 as log so $\text{pH} = -\log[\text{H}^+]$. All the rules we have looked at are the same just when the base $a = 10$ so in particular:

$$\boxed{\text{If } y = 10^x \text{ then } x = \log(y)}$$

Logarithms to the Base e

The second common logarithm found in chemistry is the logarithm to the base e known as the 'natural logarithm'. We use the notation $\ln(x)$ but this means the same as $\log_e(x)$. The natural logarithm is the inverse operation for the exponential ($y = e^x$) so we have the relationship as before:

$$\boxed{\text{If } y = e^x \text{ then } x = \ln(y)}$$

Example:

If $3 = e^x$ then $x = \ln 3 \approx 1.09861$

As natural logarithms are the inverse operation to exponentials ($y = e^x$) we have the following rules:

$$\boxed{\ln(e^x) = x}$$

$$\boxed{e^{\ln(x)} = x}$$

Note: This rules are the same as the more general ones earlier in the section however look different due to the ln notation.

Example:

We can simplify $e^{\ln(x^4+2)} = x^4+2$.

Example:

We can simplify $\ln\left(e^{(5x^4+2^x)}\right) = 5x^4 + 2^x$.

Laws of Logarithms

There are 3 laws of logarithms that we use to help algebraically manipulate logarithms:

1. $\log_a(x \times y) = \log_a(x) + \log_a(y)$
2. $\log_a\left(\dfrac{x}{y}\right) = \log_a(x) - \log_a(y)$
3. $\log_a(x^b) = b \times \log_a(x)$

Note: Remember we write $\ln(x)$ for $\log_e(x)$.

Example: Simplify each of the following into a single logarithm:

1. $\log 5 + \log 2$
2. $\log_3 2 + \log_3 2 + \log_3 2$
3. $3\log 3 - 2\log 2$
4. $\ln 8 - \ln 4$

Solution:

1. Using the first law we can see that:
$$\log 5 + \log 2 = \log 5 \times 2 = \log 10.$$
Since log is used to denote the base 10 logarithm, $\log 10 = 1$
2. This can be done using law 1 or by using law 3:
$$\log_3 2 + \log_3 2 + \log_3 2 = 3\log_3 2 = \log_3 2^3 = \log_3 8$$
3. Law 3 needs to be used to remove the co-efficient in front of the logs:
$$3\log 3 - 2\log 2 = \log 3^3 - \log 2^2 = \log 27 - \log 4.$$
Now law 2 is applied to produce, $\log \frac{27}{4}$ which can't be simplified further.
4. Law 2 is used to give:
$$\ln 8 - \ln 4 = \ln \tfrac{8}{4} = \ln 2$$

Chemistry Example: A general reaction takes place of the form:

$$a\,\mathrm{A} + b\,\mathrm{B} \longrightarrow c\,\mathrm{C} + d\,\mathrm{D}$$

where the equilibrium constant K is defined as $K = [\mathrm{A}]^{-a} \times [\mathrm{B}]^{-b} \times [\mathrm{C}]^{c} \times [\mathrm{D}]^{d}$. Find the logarithm of K as a sum of logarithms.

Solution: First we take the log of both sides of the equation.

$$\log K = \log\left([\mathrm{A}]^{-a} \times [\mathrm{B}]^{-b} \times [\mathrm{C}]^{c} \times [\mathrm{D}]^{d}\right)$$

Then using law 1 we can expand this to be a sum of several logs.

$$\log K = \log\left([\mathrm{A}]^{-a}\right) + \log\left([\mathrm{B}]^{-b}\right) + \log\left([\mathrm{C}]^{c}\right) + \log\left([\mathrm{D}]^{d}\right)$$

Now we can use law 3 to bring the powers down.

$$\log K = -a\log[\mathrm{A}] - b\log[\mathrm{B}] + c\log[\mathrm{C}] + d\log[\mathrm{D}]$$

Converting between Logarithms to Different Bases

We may wish to convert between the different logarithms of different bases so for example we might want to convert $\log(x)$ to $\ln(x)$. We do this using the following formula:

$$\boxed{\log_a(x) = \frac{1}{\log_b(a)} \times \log_b(x)}$$

Example: Convert $\log(x)$ to be in the form $\ln(x)$

Solution: Remember that $\log(x) = \log_{10}(x)$ and $\ln(x) = \log_e(x)$. So using the formula above we have:

$$\log_{10}(x) = \frac{1}{\log_e(10)} \times \log_e(x)$$
$$\Longrightarrow \log_{10}(x) = \frac{\ln(x)}{\ln(10)}$$

2.6 Rearranging Exponentials and Logarithms

When working with logarithms and exponentials the same rules for rearranging apply. We still use **BODMAS** in reverse order and the logarithms and exponentials are rearranged at the **O**rders stage. There are two rules that we utilise when rearranging these equations:

1. $a^{\log_a x} = x$
2. $\log_a(a^x) = x$

This also works if we are using ln instead of log; it's just a different notation.

Note: When exponentiating or taking a logarithm we must do the operation to the *whole* side of the equation.

Example: Make x the subject in the following equations:

1. $y = 10^x - 1$
2. $\ln(x+2) = \ln(y) + \ln(2)$

Solution:

1. As we are doing **BODMAS** in reverse we start by adding 1 to both sides:

$$\begin{aligned} y + 1 &= 10^x && \text{Take a logarithm of base 10 of both sides} \\ \log_{10}(y+1) &= \log_{10}(10^x) && \text{The right hand side simplifies to } x \\ x &= \log_{10}(y+1) \end{aligned}$$

2. We can use the laws of logarithms to get the right hand side all as one natural logarithm:

$$\begin{aligned} \ln(x+2) &= \ln(2y) && \text{Exponentiate both sides} \\ e^{\ln(x+2)} &= e^{\ln(2y)} && \text{Simplify this} \\ x + 2 &= 2y && \text{Subtract 2 from both sides} \\ x &= 2y - 2 \end{aligned}$$

Chemistry Example: Rearrange the pH equation, $\text{pH} = -\log_{10}[\text{H}^+]$, so that $[\text{H}^+]$ is the subject of the formula.

Click here for a video example

Solution: First we use the third of logarithms to get:

$$\text{pH} = \log_{10}\left([\text{H}^+]^{-1}\right).$$

We now take exponentials to the base 10 of both sides of the equation.

$$10^{\text{pH}} = 10^{\log_{10}[\text{H}^+]^{-1}}$$

Logarithms and exponentials to the same base cancel.

$$\begin{aligned} 10^{\text{pH}} &= [\text{H}^+]^{-1} \\ \implies 10^{\text{pH}} &= \frac{1}{[\text{H}^+]} \\ \implies [\text{H}^+] &= \frac{1}{10^{\text{pH}}} \\ \implies [\text{H}^+] &= 10^{-\text{pH}} \end{aligned}$$

Chemistry Example: Rearrange the Arrhenius equation

$$k = A\exp\left(-\frac{E_a}{RT}\right)$$

so that T is the subject of the formula.

Click here for a video example

Solution: First we need to divide both sides of the equation by A.

$$\frac{k}{A} = \exp\left(-\frac{E_a}{RT}\right)$$

The inverse of the exponential function is the natural logarithm. So we must take the natural logarithm of both sides of the equation:

$$\ln\left(\frac{k}{A}\right) = \ln\left(\exp\left(-\frac{E_a}{RT}\right)\right).$$

Logarithms and exponentials to the same base cancel.

$$\ln\left(\frac{k}{A}\right) = -\frac{E_a}{RT}$$

$$\implies T\ln\left(\frac{k}{A}\right) = -\frac{E_a}{R}$$

$$\implies T = -\frac{E_a}{R\ln\left(\frac{k}{A}\right)}$$

2.7 Simultaneous Equations

The simplest simultaneous equations are two equations with two variables. They are called simultaneous because they must both be solved at the same time to find a pair of numbers that satisfy both equations. The two equations below form a pair simultaneous of equations:

$$2y - x = 1 \quad (1)$$
$$x + y = 5 \quad (2)$$

In order to solve these we use a method called substitution shown in the example below. We start by making one of the variables the subject of one of the equations. We then substitute this new expression into the other equation and solve.

Note: Similar methods can be applied to 3 equations with 3 unknowns and more generally for n equations with n unknowns.

Example: Solve the simultaneous equations: $y + x = 5$ (1) and $2y - x = 1$ (2).

Solution: To solve these we will make one of the variables the subject. Take equation (2) and make x the subject:

$$2y = x + 1$$
$$\implies 2y - 1 = x$$

Note: We could have found y as the subject or used equation (1) it does not matter!
As $x = 2y - 1$ we can **substitute** this expression into (1) to get that: (We must always substitute our expression into the other equation that we did not rearrange in the step before).

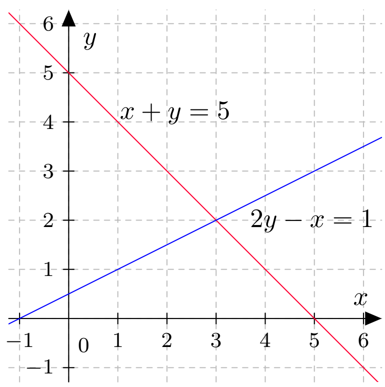
$$y + x = 5$$
$$\implies y + (2y - 1) = 5$$
$$\implies 3y - 1 = 5$$
$$\implies 3y = 6$$
$$\implies y = 2$$

We have the value of $y = 2$. To find out what x is we need to **substitute** $y = 2$ into either one of the equations (both should give you the same answer). So if we substitute this into (1) we get:

$$y + x = 5$$
$$\implies 2 + x = 5$$
$$\implies x = 3$$

We have the solution of $x = 3$ and $y = 2$.

Solving these simultaneous equations can also be done graphically. Below are both equations plotted on the same graph. Notice the intersection point of the lines is (3,2) which is what we calculated.



Example: Stacy's mother was 30 years old when she was born. At what age is she half her mother's age?

Solution: To solve this problem we first need to form equations that describe the information given to us. Let the variables s and m denote the age of Stacy and her mother respectively then we can write:

1 $m = s + 30$ Meaning that Stacy's mother is 30 years older than her.

2 $s = \frac{1}{2}m$ Meaning that Stacy's age is half her mother's.

We want to find Stacy's age s so to do that we shall substitute 1 into 2 resulting in:

$$\begin{aligned} s &= \tfrac{1}{2}(s+30) && \text{Multiply each side by 2} \\ 2s &= s + 30 && \text{Subtract } s \text{ from both sides} \\ s &= 30 \end{aligned}$$

Stacy will be 30 when she's half her mother's age.

Chemistry Example: Results from a mass spectrometry experiment show that 2 fragments of a molecule both contain hydrogen and carbon. The empirical formula for the first fragment is C_2H_5 which has a mass of 29 amu and the second has a formula of C_8H_{18} with a mass of 114 amu. Calculate the mass of the carbon and hydrogen atoms.

Solution: First we write the information provided in equations. We shall use the variables C and H to be the mass of the carbon and hydrogen respectively. For the first fragment we can write $2\mathrm{C}+5\mathrm{H} = 29$ and for the second fragment $8\mathrm{C}+18\mathrm{H} = 114$. So we have the simultaneous equations:

$$\begin{aligned} 2\mathrm{C} + 5\mathrm{H} &= 29 && (1) \\ 8\mathrm{C} + 18\mathrm{H} &= 114 && (2) \end{aligned}$$

To solve these we use substitution. In 1 we make C the subject by first subtracting 5 H from both sides to give:

$$2\,\mathrm{C} = 29 - 5\,\mathrm{H} \quad (3)$$

From here we notice that in 2 there is a 8 C. We can multiply both sides of 3 by 4 to get $8\,\mathrm{C} = 116 - 20\,\mathrm{H}$ which can be substituted into 2 to give:

$$\begin{aligned} (116 - 20\,\mathrm{H}) + 18\,\mathrm{H} &= 114 \\ \implies 116 - 2\,\mathrm{H} &= 114 \\ \implies 116 - 114 &= 2\,\mathrm{H} \\ \implies 2 &= 2\,\mathrm{H} \\ \implies 1 &= \mathrm{H} \end{aligned}$$

Now that we have found H, all we need to do is put that value into one of the equations and then we solve for C. Substituted into 1 gives:

$$\begin{aligned} 2\,\mathrm{C} + 5\,\mathrm{H} &= 29 \\ \implies 2\,\mathrm{C} + 5 &= 29 \\ \implies 2\,\mathrm{C} &= 29 - 5 \\ \implies 2\,\mathrm{C} &= 24 \\ \implies C &= 12 \end{aligned}$$

Chemistry Example: A molecule of N_2 has a mass of 4.6×10^{-26} kg and is at a temperature of 293 K. The nitrogen's velocity is given in the equation:

$$(1)\ E_k = \frac{1}{2}mv^2$$

and it's kinetic energy is given by:

$$(2)\ E_k = \frac{3}{2}k_bT$$

What is the velocity of a nitrogen molecule? ($k_b = 1.4 \times 10^{-23}$)

Solution: Considering the variables there are only 2 unknowns, E_k and v. So we have a pair of simultaneous equations. The first thing is to substitute the expression for E_k (2) into (1).

$$\begin{aligned} E_k &= \frac{1}{2}mv^2 \\ \implies \frac{3}{2}k_bT &= \frac{1}{2}mv^2 \quad (3) \end{aligned}$$

We then re-arrange (3) to make v the subject:

$$\begin{aligned} \frac{3}{2}k_bT &= \frac{1}{2}mv^2 && \text{Multiply each side by 2.} \\ 3k_bT &= mv^2 && \text{Divide by } m \text{ on both sides.} \\ \frac{3k_bT}{m} &= v^2 && \text{Finally square root.} \\ \sqrt{\frac{3k_bT}{m}} &= v \end{aligned}$$

We can now put the numbers in on the left hand side and find that $v = 520\ \text{ms}^{-1}$ (to 2 s.f.)

2.8 Quadratics

A quadratic (in the variable x) is any expression of the form:

$$\boxed{ax^2 + bx + c}$$

where a, b and c are constants. It is called a quadratic because it contains terms in x up to and including x^2.

A quadratic function has the form:

$$\boxed{y = ax^2 + bx + c}$$

where a, b and c are constants. There are a number of examples of such functions illustrated in the pages that follow.

Expanding Brackets to Produce a Quadratic

Quadratic expressions can also be factorised and written in the form:

$$(x + A)(x + B)$$

where A and B are constants. We have a method called **FOIL** of expanding quadratic equations in the above form so that they appear in the form $ax^2 + bx + c$.

FOIL stands for **F**irst, **O**uter, **I**nner and **L**ast and tells us which terms to take the product of. In the general case $(x + A)(x + B)$ **FOIL** works as follows:

1. The **F**irst terms will be the x's since they are both first in their brackets.
2. The **O**uter terms will be x and B because they are on the outer side (nearest to the edges).
3. The **I**nner terms are A and the other x for the same reason.
4. The **L**ast terms are A and B because they are last in their brackets.

We then expand our quadratic $(x + A)(x + B)$ as shown below:

$$(x + A)(x + B) = \overbrace{x \times x}^{\text{F}} + \overbrace{x \times B}^{\text{O}} + \overbrace{A \times x}^{\text{I}} + \overbrace{A \times B}^{\text{L}} = x^2 + (A + B)x + AB$$

Note: This is in the form $ax^2 + bx + c$ where $a = 1$, $b = A + B$ and $c = AB$.

Example: Expand the brackets of the following:

1. $(x + 5)(x + 7)$
2. $(x - 3)(x + 2)$
3. $(x + 1)^2$

Solution:

1. We use **FOIL** to get $(x + 5)(x + 7) = \overbrace{x \times x}^{\text{F}} + \overbrace{x \times 7}^{\text{O}} + \overbrace{5 \times x}^{\text{I}} + \overbrace{5 \times 7}^{\text{L}}$.

   Multiplying these out gives $x^2 + 7x + 5x + 35 = x^2 + 12x + 35$
2. There are some negative numbers here so be careful when using **FOIL**.

   $(x - 3)(x + 2) = \overbrace{x \times x}^{\text{F}} + \overbrace{x \times 2}^{\text{O}} + \overbrace{-3 \times x}^{\text{I}} + \overbrace{-3 \times 2}^{\text{L}} = x^2 + 2x - 3x - 6 = x^2 - x - 6$
3. We can rewrite $(x + 1)^2$ as $(x + 1)(x + 1)$ which we can then **FOIL**.

   $(x + 1)(x + 1) = \overbrace{x \times x}^{\text{F}} + \overbrace{x \times 1}^{\text{O}} + \overbrace{1 \times x}^{\text{I}} + \overbrace{1 \times 1}^{\text{L}} = x^2 + x + x + 1 = x^2 + 2x + 1$

2.9 Solving Quadratic Equations

Solving a quadratic equation involves finding all possible values of x that satisfy $ax^2 + bx + c = 0$. The values of x that satisfy this equation are called the roots.

Note that when $a = 0$, the quadratic equation reduces to a simple linear equation $bx + c = 0$ which is easy to solve. Also, when $a \neq 0$ we can divide throughout by a to get an equivalent equation of the form $x^2 + bx + c = 0$.

There are three methods that can be used to solve a quadratic:

1. Completing the square.
2. Inspection.
3. The quadratic formula.

Completing the Square

When a quadratic is in the form $x^2 + 2bx + b^2$ it is known as a perfect square because it can be factorised into a squared linear term $(x + b)^2$. However when a quadratic is not a perfect square we do have the relationship below:

$$\boxed{x^2 + 2bx + c = (x + b)^2 + (c - b^2)}$$

(To see this simply expand out the left hand side.)

Hence if we are trying to solve $x^2 + 2bx + c = 0$ then we can rewrite this as $(x + b)^2 + (c - b^2) = 0$ and then rearrange to find x.

Example: Find the values of x that make $x^2 + 4x - 1 = 0$.

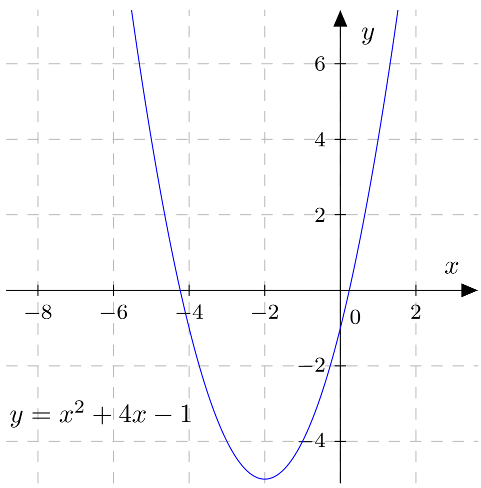
Solution: We can see that $2b = 4$ and $c = -1$ so from the equation mentioned above we can change the quadratic into the form with a perfect square:

$$\begin{aligned} x^2 + 4x - 1 &= 0 \\ \implies (x + 2)^2 + (-1 - (2^2)) &= 0 \\ \implies (x + 2)^2 - 5 &= 0 \end{aligned}$$

We can now re-arrange and take the square root of both sides:

$$\begin{aligned} &\implies (x + 2)^2 = 5 \\ &\implies x + 2 = \pm\sqrt{5} \\ &\implies x = -2 \pm \sqrt{5} \end{aligned}$$

Note: When we take the square root of both sides we need to remember that both $(-\sqrt{5})^2$ and $(-\sqrt{5})^2$ are equal to 5; the expression $\pm\sqrt{5}$ indicates that both signs are included. The two different roots for this equation are shown on the graph below.



The x-axis is where $y = 0$ so the points where the curve crosses the x-axis are the roots (where $x^2 + 4x - 1 = 0$). The graph goes through a point just to the left of $x = -4$ and just to the right of $x = 0$. Those correspond to $x = -2 - \sqrt{5}$ and $x = -2 + \sqrt{5}$ respectively.

Note: When solving a quadratic equation that has come from a scientific situation, there may be non-mathematical reasons for disregarding, say, a negative root as it might not make physical sense. A good example would be if the roots represented a time since a having negative time doesn't make sense.

Solving by Inspection

If we have a quadratic with integer coefficients it is sometimes possible to solve it by inspection. So if the quadratic $x^2 + bx + c$ can be factorised to give $(x + A)(x + B)$ we have the roots of the equation are $-A$ and $-B$. We have the following rules for solving by inspection:

- c will be the product of A and B
- b will be the sum of A and B.

In other words if we are trying to solve $x^2 + bx + c = 0$ then we need to find two numbers A and B such that their sum is b and product is c. We can then write the equation as $(x + A)(x + B) = 0$ and our roots will be $x = -A$ and $x = -B$.

Example: Find x by inspection in the following $x^2 + 5x + 6 = 0$.

Click for a video example

Solution: Since we want to factorise this we need to find two numbers that add to 5 and multiply to 6. The best way to do this is to think about what the factors of 6 are. We have 1 and 6 as well as 2 and 3. We can instantly see that $2 + 3 = 5$ so these are the numbers required. We can rewrite the original equation as:

$$x^2 + 5x + 6 = (x + 2)(x + 3)$$
$$\implies (x + 2)(x + 3) = 0$$

Now that we have the quadratic factorised we can now find out what x is. We notice if either of the terms in the brackets is 0 then the whole thing will be 0. This gives the two situations:

$$x + 2 = 0$$
$$\text{OR}$$
$$x + 3 = 0$$

When we find out what x is for each of those we see that the roots are -2 and -3. These are both solutions to this quadratic equation.

Inspection with Negative Coefficients

Inspection is easy when all the coefficients are positive but when they are negative you need to consider a few things. First if c is negative then one of A or B will be negative. This is because when a negative number multiplies a positive number the result will be negative. Secondly you would look at b, if it is positive then the larger number of A and B is positive and vice versa.

Take the example $x^2 - 4x - 5$. We first look at what factors 5 has: here the only factors are 1 and 5. Then we notice that since c is negative (here it is -5), one of A and B is negative and one is positive. Finally, since $b = -4$ is negative the sum $A + B$ is negative and this forces us to choose $A = -5$ and $B = 1$ giving us, $x^2 - 4x - 5 = (x - 5)(x + 1)$.

Example: Factorise the following:

1. $x^2 + 4x - 12$
2. $x^2 - 6x - 40$

Solution:

1. From the signs we can deduce that one of A or B is negative and, since $b = 4$, $A + B = 4$, i.e. is positive. The factors of 12 are 1 and 12, 2 and 6 and 3 and 4. The pair of numbers that we need are therefore $A = 6$ and $B = -2$ giving us $x^2 + 4x - 12 = (x + 6)(x - 2)$.
2. The signs tell us that one of A or B is negative and, since $b = -6$, $A + B = -6$, i.e. is negative. Looking at the factors of 40 we can see that -10 and 4 would produce the required result (-10 + 4 = -6) giving us, $x^2 - 6x - 40 = (x - 10)(x + 4)$.

Finally, if c is positive but b negative then both A and B have to be negative, since they would give a positive product but a negative sum.

Example: Factorise $x^2 - 8x + 15$.

Solution: Since $c = 15$ is positive we know that both A and B have the same sign and, since $b = -8$, $A + B = -8$, we see that they must both be negative. Looking at the factors of 15 we can see that -5 and -3 would produce the required result (-5 - 3 = -8) giving us, $x^2 - 8x + 15 = (x - 5)(x - 3)$.

The Quadratic Formula

If all else fails we can always rely on the quadratic formula. If we have a quadratic equation of the form $ax^2 + bx + c = 0$ then the quadratic formula for the roots is:

$$\boxed{x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}}$$

Note: The $\pm$ symbol means plus or minus. So we have two solutions one for when you add the square root and one where you subtract.

Example: Use the quadratic formula to solve the quadratic equation $3x^2 - 5x + 2$

Solution: As we are using the formula all we need to do is put in the values for a, b and c. So $a = 3$, $b = -5$ and $c = 2$. Putting these into the equation yields:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{-(-5) \pm \sqrt{(-5)^2 - 4(3 \times 2)}}{2 \times 3}$$

$$\implies x = \frac{5 \pm \sqrt{25 - 24}}{6}$$

$$\implies x = \frac{5 \pm \sqrt{1}}{6}$$

$$\implies x = \frac{5 + 1}{6} = 1 \qquad \text{corresponding to the positive square root } +\sqrt{1}$$

$$\implies x = \frac{5 - 1}{6} = \frac{4}{6} = \frac{2}{3} \qquad \text{corresponding to the negative square root } -\sqrt{1}$$

So $x = 1$ and $x = \frac{2}{3}$ are the two roots.

Chemistry Example: Formic acid is a weak acid with a dissociation constant K_a of 1.8×10^{-4}. The K_a relates the concentration of the H^+ ions denoted $[H^+]$ and the amount of acid dissolved denoted N by the equation:

$$K_a = \frac{[H^+]^2}{N - [H^+]}$$

Given that there is 0.1 moles of formic acid dissolved, calculate the pH of the solution.

Solution: To find the pH first we need to find the concentration of H^+ ions. Lets start by re-arranging the equation for K_a.

$$\begin{aligned} K_a &= \frac{[H^+]^2}{N - [H^+]} && \text{Multiply both sides by } (N - [H^+]) \\ \implies K_a(N - [H^+]) &= [H^+]^2 && \text{Expand the bracket} \\ \implies K_aN - K_a[H^+] &= [H^+]^2 && \text{Take everything over to one side} \\ \implies 0 &= [H^+]^2 + K_a[H^+] - K_aN \end{aligned}$$

The equation $[H^+]^2 + K_a[H^+] - K_aN = 0$ is quadratic as K_a and N are constants and our variable (usually denoted x) is $[H^+]$.

We will put the symbols K_a and N into the quadratic formula and then put the numbers in afterwards to avoid complicating things. So as $a = 1$, $b = K_a$ and $c = -K_aN$ we have:

$$[H^+] = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{-K_a \pm \sqrt{{K_a}^2 - 4(-K_aN)}}{2}$$

$$\implies [H^+] = \frac{-K_a \pm \sqrt{{K_a}^2 + 4K_aN}}{2}$$

Putting the numbers given into that equation gives $[H^+] = 4.15\ldots \times 10^{-3}$ for the positive square root and $[H^+] = -4.33\ldots \times 10^{-3}$ for the negative square root. We can immediately disregard the negative answer because you can't have a negative concentration of H^+.

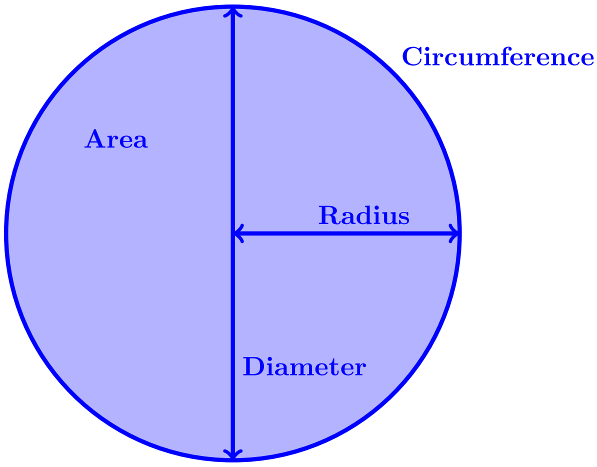
The final stage is to calculate the pH using the pH formula $\text{pH} = -\log[H^+]$.

$$\text{pH} = -\log(4.15 \times 10^{-3}) = 2.38\ldots \text{ So pH} = 2.4 \text{ (to 2 s.f.).}$$

3 Geometry and Trigonometry

3.1 Geometry

Circles: Area, Radius, Diameter and Circumference



Above we have a circle which shows the Area A, Radius r, Diameter d and Circumference C of a circle. These are related by the following equations:

- $d = 2r$
- $A = \pi r^2$
- $C = 2\pi r$

Note: π is the number $3.14159\ldots$ which relates the circumference to the diameter $\pi = \frac{C}{d}$. It has an infinite number of decimal places that do not repeat.

Chemistry Example: A hydrogen atom has a diameter of 106 pm. For a circle with a diameter of 106 pm calculate the:

1. Circumference.
2. Area.

Solution:

1. To find the circumference first we must find the radius.

$$d = 2r \Rightarrow r = \frac{d}{2}.\text{ So } r = \frac{106\text{ pm}}{2} = 53.0\text{ pm}.$$

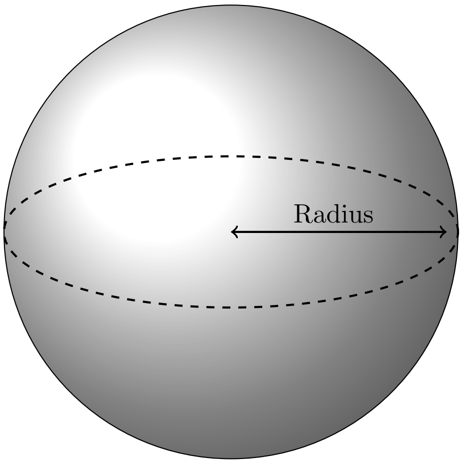
Now we can find the circumference by using:

$$C = 2\pi r = 2\pi \times 53.0\text{ pm} = 333.00\ldots\text{ pm} = 333\text{pm (to 3 s.f.)}.$$

2. As we know $r = 53.0$ pm we can find the area.

$$A = \pi r^2 = \pi \times (53.0\text{ pm})^2 = \pi \times 2.809 \times 10^{-21}\text{ m} = 8.824\ldots \times 10^{-21}\text{ m}$$
$$= 8.82 \times 10^{-21}\text{ m (to 2 s.f.)}.$$

Spheres: Volume and Surface Area



Above we have a picture that shows the radius of a sphere which is the distance from the centre to the surface. The volume V of a sphere is given by:

$$V = \frac{4\pi r^3}{3}$$

and the surface area A_S is given by:

$$A_S = 4\pi r^2$$

Chemistry Example: A flourine atom is measured to have a radius of 53 pm. For a sphere with a radius of 53 pm calculate the:

1. Volume.
2. Surface area.

Solution:

1. As $r = 53$ pm we can find the volume by using the formula:

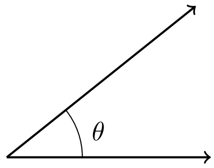
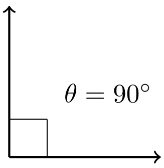
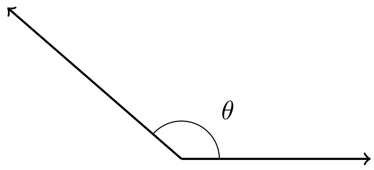
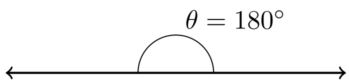
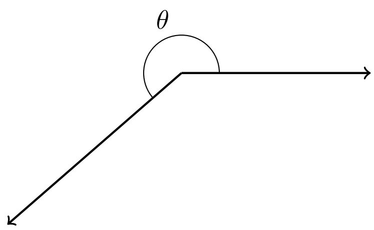
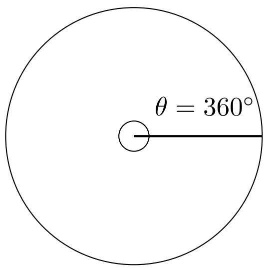
$$V = \frac{4\pi r^3}{3} = \frac{4\pi \times (53 \text{ pm})^3}{3} = \frac{4\pi \times 1.489 \times 10^{-31}\text{m}^3}{3} = 6.24 \times 10^{-31} \text{ m}^3 \text{ (to 3 s.f.)}.$$

2. We can find the surface area by using the formula:

$$A_S = 4\pi r^2 = 4\pi \times (53 \text{ pm})^2 = 4\pi \times 2.809 \times 10^{-21} \text{ m}^2 = 3.53 \times 10^{-20} \text{ m}^2 \text{ (to 3 s.f.)}.$$

3.2 Trigonometry

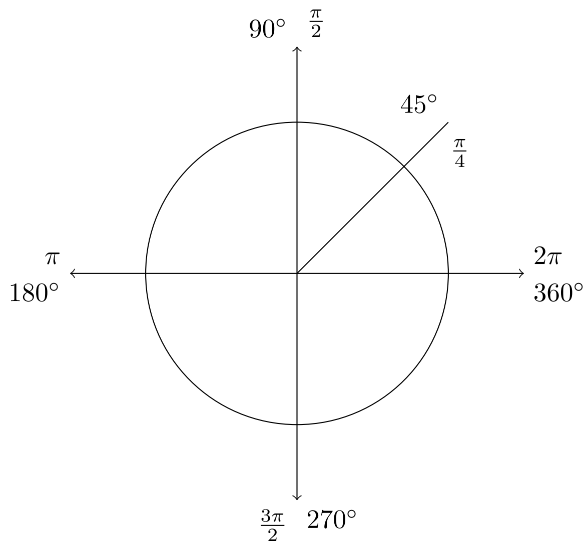
Angles

Angle Type	Size of Angle	Angle Example
Acute Angle	$0^\circ < \theta < 90^\circ$	
Right angle	$\theta = 90^\circ$	
Obtuse angle	$90^\circ < \theta < 180^\circ$	
Straight line	$\theta = 180^\circ$	
Reflex angle	$180^\circ < \theta < 360^\circ$	
Full circle	$\theta = 360^\circ$	

Radians

We often use degrees to measure angles however we have another measurement of angles called radians. Instead of splitting a full circle into $360°$, it is split into 2π radians. We must use radians in calculus (differentiation and integration), complex numbers and polar coordinates. This may seem new and complicated at first however it is no different to thinking that we could measure length in miles or metres.

Below we have a full circle showing some angles in degree and what they are in radians.



We may wish to convert between degree and radians. In order to turn $x°$ degrees into radians we use the formula:

$$\boxed{\frac{x°}{360°} \times 2\pi}$$

In order to convert x radians into degrees we use the formula:

$$\boxed{\frac{x}{2\pi} \times 360°}$$

Example: Convert the following:

1. $60°$ into radians.
2. $\frac{3\pi}{8}$ radians into degrees.

Solution:

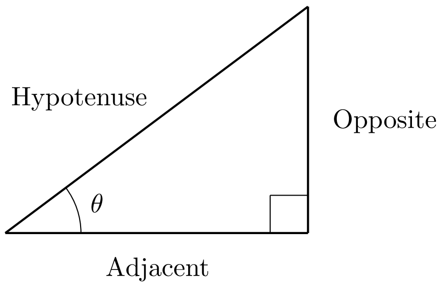
1. We need to use the formula $\frac{x°}{360°} \times 2\pi$

$$\frac{x°}{360°} \times 2\pi = \frac{60°}{360°} \times 2\pi = \frac{\pi}{3} \text{ radians.}$$

2. We need to use the formula $\frac{x}{2\pi} \times 360°$.

$$\frac{x}{2\pi} \times 360° = \frac{\left(\frac{3\pi}{8}\right)}{2\pi} \times 360° = \frac{3}{16} \times 360° = 67.5°$$

Right-Angled Triangles



As shown in the diagram above when given a right-angled triangle with one of the non-right angles labelled θ then we label the sides as follows:

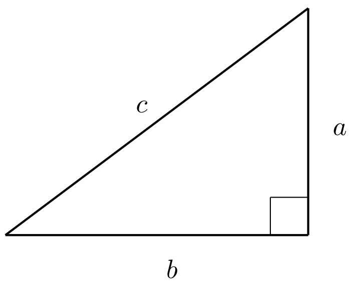
- The longest side is called the **hypotenuse** this is always the side opposite the right angle.
- The side that is opposite the angle θ is called the **opposite**.
- The side that is next to the angle θ is called the **adjacent**.

Pythagoras' Theorem

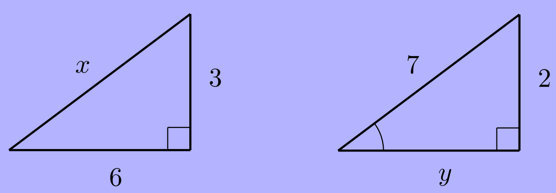
Pythagoras' theorem relates only to right-angled triangles. So given a right-angled triangle such as the one below it states:

$$c^2 = a^2 + b^2$$

where c is the length of the hypotenuse and a and b are the lengths of the other two sides of the triangle.



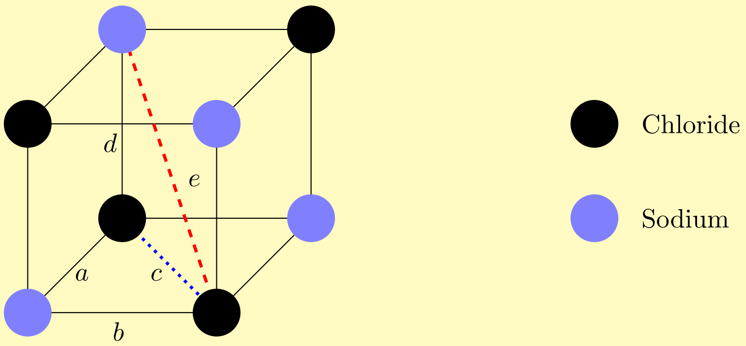
Example: Find the length of x and y in the following triangles:



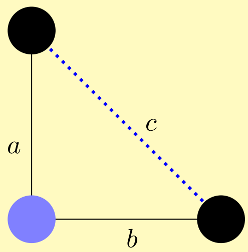
Solution:

1. Using Pythagoras' Theorem we know that, since x is the hypotenuse, $x^2 = 3^2 + 6^2 \implies x = \sqrt{45} \approx 6.708$.
2. Using Pythagoras' Theorem we know that $7^2 = y^2 + 2^2 \implies y = \sqrt{45} \approx 6.708$.

Chemistry Example: Below is the structure of solid sodium chloride. If the distance between the centres of adjacent chloride and sodium ions is 278 pm, what is the next shortest distance between such ions? i.e. what is the length of the red dashed line?

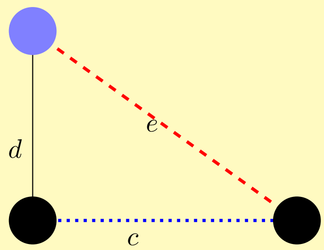


Solution: First we consider the triangle from the cube lattice above with lengths a, b, c. This is a right-angled triangle shown below so we can apply Pythagoras' Theorem.



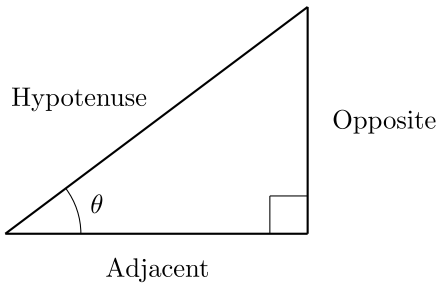
We know from the question that the distance between adjacent chloride and sodium ions is 278 pm so $a = b = 278$ pm. So we have using Pythagoras' theorem $c^2 = 278^2 + 278^2 \implies c = 393$ pm.

Now consider the triangle from the cube lattice with lengths c, d, e. This is a right-angled triangle shown below so we can again apply Pythagoras' Theorem.



We know from the question that the distance between adjacent chloride and sodium ions is 278 pm so $d = 278$ pm and from our previous calculations we know $c = 393$ pm. So we have using Pythagoras' theorem $e^2 = 278^2 + 393^2 \implies e = 481$ pm.

SOHCAHTOA



Given our right-angled triangle we start by defining sine, cosine and tangent before reviewing what their graphs look like.

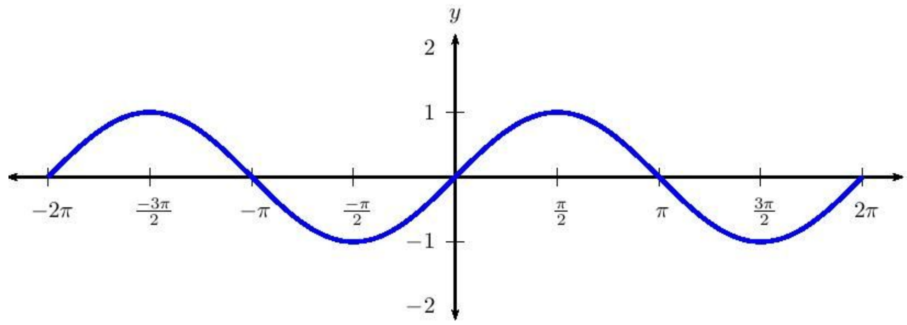
Note: The angle θ is measured in radians in the following graphs on the x-axis.

Sine Function

We define sine as the ratio of the opposite to the hypotenuse.

$$\sin(\theta) = \frac{\text{Opposite}}{\text{Hypotenuse}}$$

Part of the graph of $y = \sin(\theta)$ is shown below.

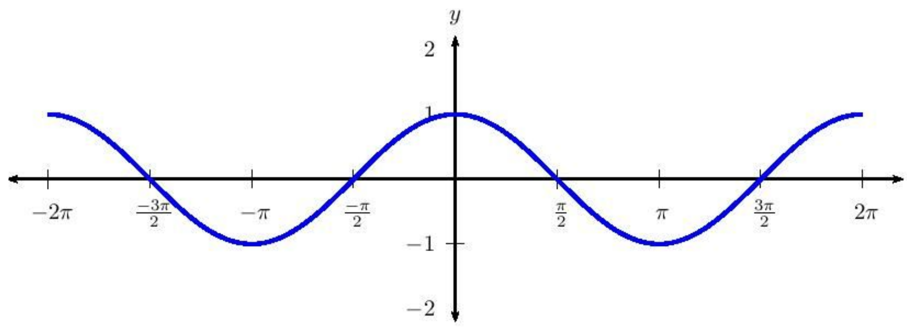


Cosine Function

We define cosine as the ratio of the adjacent to the hypotenuse.

$$\cos(\theta) = \frac{\text{Adjacent}}{\text{Hypotenuse}}$$

Part of the graph of $y = \cos(\theta)$ is shown below.



Tangent Function

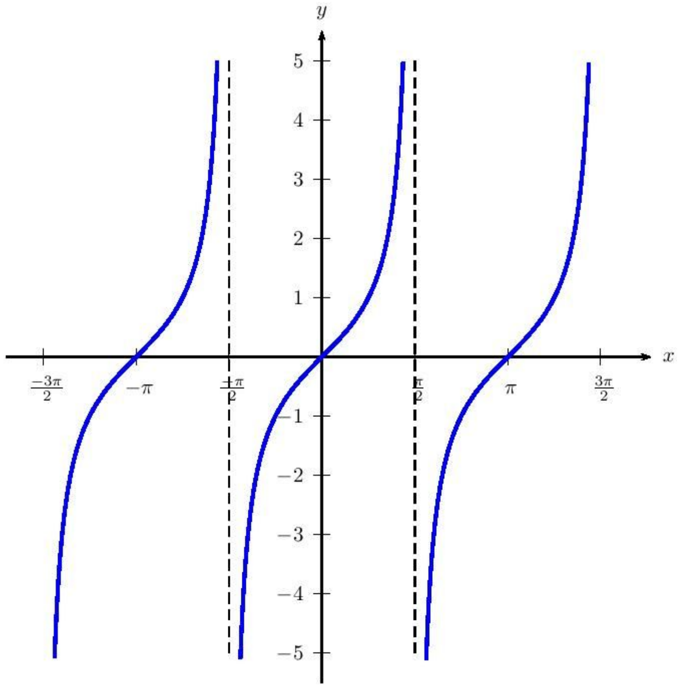
We define tangent as the ratio of the opposite to the adjacent.

$$\tan(\theta) = \frac{\text{Opposite}}{\text{Adjacent}}$$

This leads to the relationship $\tan(\theta) = \dfrac{\sin(x)}{\cos(x)}$ shown below:

$$\tan(\theta) = \frac{\text{Opposite}}{\text{Adjacent}} = \frac{\text{Opposite } \times \text{ Hypotenuse}}{\text{Adjacent } \times \text{ Hypotenuse}} = \frac{\left(\dfrac{\text{Opposite}}{\text{Hypotenuse}}\right)}{\left(\dfrac{\text{Adjacent}}{\text{Hypotenuse}}\right)} = \frac{\sin(x)}{\cos(x)}$$

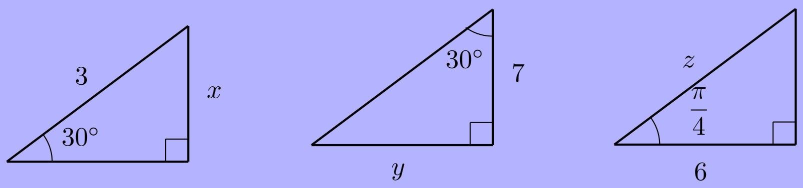
The graph of $y = \tan(\theta)$ is shown below.



The definitions of sine, cosine and tangent are often more easily remembered by using SOHCAHTOA. We can use the formulas in SOHCAHTOA to calculate the size of angles and the length of sides in **right-angled triangles**.

$$\underbrace{\text{S O H}}_{\sin(\theta)=\frac{\text{Opposite}}{\text{Hypotenuse}}}\ \underbrace{\text{C A H}}_{\cos(\theta)=\frac{\text{Adjacent}}{\text{Hypotenuse}}}\ \underbrace{\text{T O A}}_{\tan(\theta)=\frac{\text{Opposite}}{\text{Adjacent}}}$$

Example: Using SOHCAHTOA find the lengths x, y and z in the right-angled triangles below.



Solution: For shorthand we have used H to denote the hypotenuse, O the opposite and A the adjacent.

1. We know the length of the hypotenuse and wish to find the opposite hence we need to use

$$\sin(\theta) = \frac{\mathrm{O}}{\mathrm{H}} \Longrightarrow \sin(30^\circ) = \frac{\mathrm{O}}{3} \Longrightarrow \mathrm{O} = \sin(30^\circ) \times 3 = \frac{3}{2}$$

   Note: This question is in degrees.

2. We know the length of the adjacent and wish to find the opposite hence we need to use

$$\tan(\theta) = \frac{\mathrm{O}}{\mathrm{A}} \Longrightarrow \tan(30^\circ) = \frac{\mathrm{O}}{7} \Longrightarrow \mathrm{O} = \tan(30^\circ) \times 7 = \frac{7\sqrt{3}}{3}$$

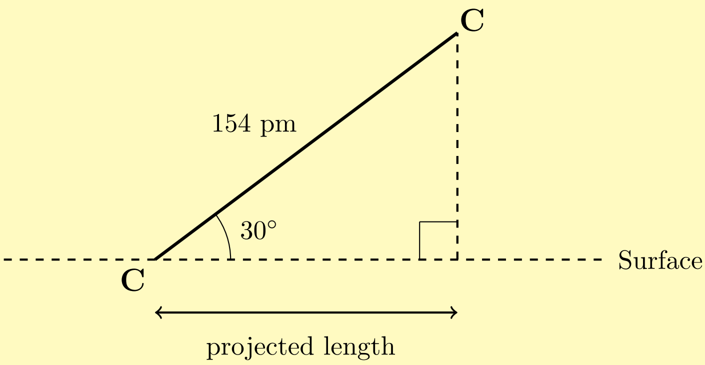
   Note: This question is in degrees.

3. We know the length of the adjacent and wish to find the hypotenuse hence we need to use

$$\cos(\theta) = \frac{\mathrm{A}}{\mathrm{H}} \Longrightarrow \cos\left(\frac{\pi}{4}\right) = \frac{6}{\mathrm{H}} \Longrightarrow \mathrm{H} = \frac{6}{\cos\left(\frac{\pi}{4}\right)} = 6\sqrt{2}$$

   Note: This question is in radians.

Chemistry Example: A carbon-carbon bond has a length of 154 pm. If the bond is positioned at an angle of 30° to a surface as shown in the picture. What is the projected length of the bond?



Solution: To solve this we should first note that we have a right-angled triangle and can therefore use SOCAHTOA. We know the hypotenuse which is 154 pm and want to find the projected length which is the adjacent. So we need to use:

$$\cos(\theta) = \frac{\mathrm{A}}{\mathrm{H}} \Longrightarrow \cos(30^\circ) = \frac{\mathrm{A}}{154 \text{ pm}} \Longrightarrow \mathrm{A} = \cos(30^\circ) \times 154 \text{ pm} = 77\sqrt{3} \text{ pm}$$

$$\Longrightarrow \text{Projected length} = 77\sqrt{3} \text{ pm} \approx 133 \text{ pm}.$$

Inverse Function and Rearranging Trigonometric Functions

We may be given the lengths of two sides of a right-angled triangle and be asked to find the angle θ between them or be asked to rearrange an equation with a trigonometric function. In order to do these we need to introduce the inverse trigonometric functions:

- The inverse function of sine $\sin(..)$ is $\sin^{-1}(..)$ also can be denoted as $\arcsin(..)$.
- The inverse function of cosine $\cos(..)$ is $\cos^{-1}(..)$ also can be denoted as $\arccos(..)$.
- The inverse function of tangent $\tan(..)$ is $\tan^{-1}(..)$ also can be denoted as $\arctan(..)$.

We use the inverse trigonometric functions with SOHCAHTOA to find the values of angles in right-angled triangles in which two of the lengths of the sides have been given. We do this as follows, suppose we know that:

$$\sin(\theta) = \frac{1}{2}$$

To find θ we can apply the inverse sine function to both sides of the equation.

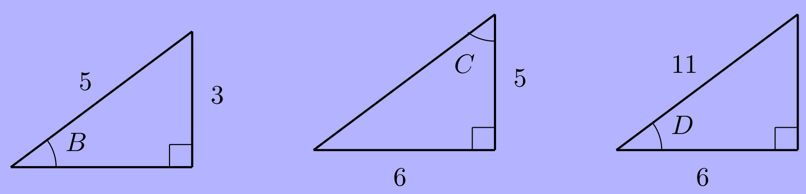
$$\sin^{-1}(\sin(\theta)) = \sin^{-1}\left(\frac{1}{2}\right).$$

$$\Longrightarrow \theta = \sin^{-1}\left(\frac{1}{2}\right).$$

$$\Longrightarrow \theta = 30^\circ.$$

We can use a calculator to find $\sin^{-1}\left(\frac{1}{2}\right) = 30^\circ$ or $\sin^{-1}\left(\frac{1}{2}\right) = \frac{\pi}{6}$ radians.

Example: Using SOHCAHTOA find the size of the angles B, C and D in the right-angled triangles below.



Solution: For shorthand we have used H to denote the hypotenuse, O the opposite and A the adjacent.

1. We know the length of the hypotenuse and the opposite.

$$\sin(\theta) = \frac{\text{O}}{\text{H}} \Longrightarrow \sin(B) = \frac{3}{5} \Longrightarrow B = \sin^{-1}\left(\frac{3}{5}\right) = 36.9^\circ \text{ or } 0.64 \text{ radians.}$$

2. We know the length of the adjacent and the opposite.

$$\tan(\theta) = \frac{\text{O}}{\text{A}} \Longrightarrow \tan(C) = \frac{6}{5} \Longrightarrow C = \tan^{-1}\left(\frac{6}{5}\right) = 50.2^\circ \text{ or } 0.88 \text{ radians.}$$

3. We know the length of the hypotenuse and the adjacent.

$$\cos(\theta) = \frac{\text{A}}{\text{H}} \Longrightarrow \cos(D) = \frac{6}{11} \Longrightarrow D = \cos^{-1}\left(\frac{6}{11}\right) = 56.9^\circ \text{ or } 0.99 \text{ radians.}$$

Note: When squaring trigonometric functions such as $(\sin(x))^2$, $(\cos(x))^2$ and $(\tan(x))^2$ we use the notation $\sin^2(x)$ for $(\sin(x))^2$; $\cos^2(x)$ and $\tan^2(x)$ are used in the same way. This is also true more generally for example $(\sin(x))^n$ is denoted by $\sin^n(x)$

Chemistry Example: The position of certain bands in the infra-red spectrum of SO_2 can be used to determine the angle θ of the O-S-O bonds. The analysis leads to the equation:

$$\sin^2\left(\frac{\theta}{2}\right) = 0.769$$

Find the value of θ in degrees.

Click here for a video example

Solution: First we can square root both sides to remove the square on the sin. This gives us:

$$\sqrt{\sin^2\left(\frac{\theta}{2}\right)} = \sqrt{0.769}$$

$$\implies \sin\left(\frac{\theta}{2}\right) = 0.8769\ldots$$

We now take the inverse sin of both sides:

$$\sin^{-1}\left(\sin\left(\frac{\theta}{2}\right)\right) = \sin^{-1}(0.8769)$$

$$\implies \frac{\theta}{2} = \sin^{-1}(0.8769)$$

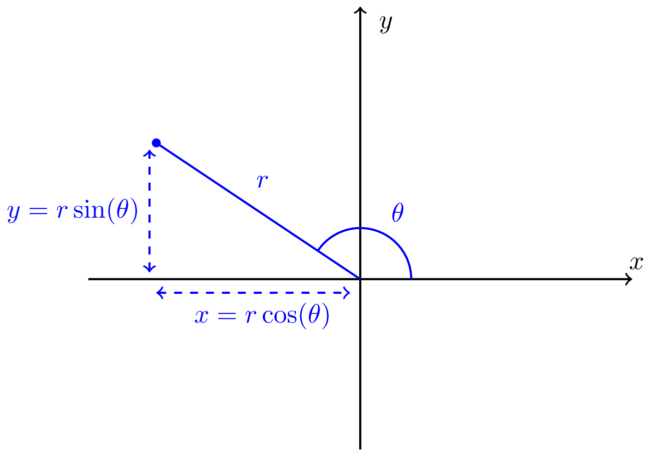
$$\implies \frac{\theta}{2} = 61.27\ldots$$

$$\implies \theta = 123^\circ \text{ (to 3 s.f.)}$$

3.3 Polar Coordinates

With the usual x, y-axis we will be familiar with coordinates in the form $(3, 2)$ meaning that we move 3 units in the x-direction (along the x-axis) followed by a move of 2 units in the y-direction. These are Cartesian coordinates.

There is another coordinate system called Polar coordinates. These are coordinates in the form (r, θ) where r is the distance to the point from the origin $(0, 0)$ and θ is the angle, in **radians**, between the positive x-axis and the line formed by r. This is all shown in the diagram below:



So the point that has Cartesian coordinates (x, y) can also be described in Polar form as (r, θ). From trigonometry and the Pythagoras theorem we have the following relationships:

- $x = r\cos(\theta)$
- $y = r\sin(\theta)$
- $r = \sqrt{x^2 + y^2}$

We can used the formulae above to allow us to convert Polar and Cartesian coordinates.

Example: A point has Polar coordinates $\left(3, \dfrac{-\pi}{4}\right)$. What are the corresponding Cartesian coordinates?

Solution: So $r = 3$ and $\theta = \dfrac{-\pi}{4}$. So using the formulae above we have:

$x = r\cos(\theta) = 3 \times \cos\left(\dfrac{-\pi}{4}\right) = \dfrac{3\sqrt{2}}{2}$

$y = r\sin(\theta) = 3 \times \sin\left(\dfrac{-\pi}{4}\right) = \dfrac{-3\sqrt{2}}{2}$

So our Cartesian coordinates are $\left(\dfrac{3\sqrt{2}}{2}, \dfrac{-3\sqrt{2}}{2}\right)$.

Example: A point has Cartesian coordinates $(-2, 3)$. What are the corresponding Polar coordinates?

Solution: So we have that $x = -2$ and $y = 3$. So using the formulae above we have:

$r = \sqrt{x^2 + y^2} = \sqrt{(-2)^2 + 3^2} = \sqrt{13}$

Now we we can find θ.

$x = r\cos(\theta) \Rightarrow \theta = \cos^{-1}\left(\frac{x}{r}\right) = \cos^{-1}\left(\frac{-2}{\sqrt{13}}\right) = 2.158\cdots = 2.16$ radians

So our Polar coordinates are $(\sqrt{13}, 2.16)$.

4 Differentiation

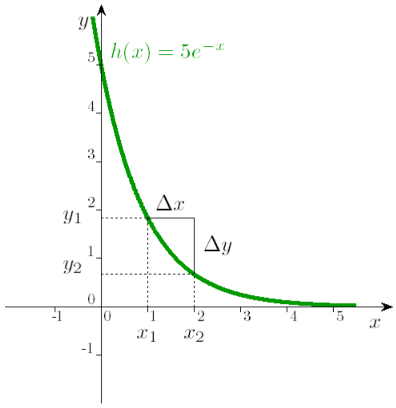
4.1 Introduction to Differentiation

Recall the equation of a straight line is of the form of $y = mx + c$ where m is the gradient and c is the intercept. We can find the gradient m of a straight line using the triangle method with the formula $m = \frac{\Delta x}{\Delta y}$.

Note: Remember that the gradient is a measure of how steep the graph is a certain point.

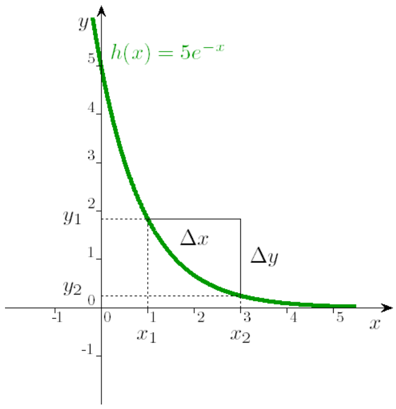
As the gradient of a straight line is the same at every point on the line it is easy to find. With a curve this is not the case. Consider the graph of $y = 5e^{-x}$ shown below we will use the triangle method with two different triangles and show we get two different values for the gradient.

Using the triangle method with the triangle in the graph below gives:



$$\text{gradient} = \frac{\Delta y}{\Delta x} = \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{y_2 - y_1}{x_2 - x_1} = \frac{0.68 - 1.85}{3 - 1} = -1.17$$

Now if we use the triangle method again but this time with a larger triangle as in the graph below:



$$\text{gradient} = \frac{\Delta y}{\Delta x} = \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{y_2 - y_1}{x_2 - x_1} = \frac{0.25 - 1.85}{3 - 1} = -0.8$$

We have two different values for the gradient of the curve. This is because the value of the gradient is not the same at all points on the curve, unlike a straight line. This should be obvious as we can see that the steepness of the graph changes along the curve. This means it is quite hard to find the gradient of a curve using the triangle method and so we need a new method.

Differentiation allows us to find the gradient of a graph. The reason that this works is because when we differentiate we are calculating how one variable changes due to a change in another (in other words the rate of change). This is useful in chemistry: for example we might wish to know how the concentration of a reactant $[OH^-]$, changes with time t.

Notation

When we use the triangle method we are finding $\frac{\Delta y}{\Delta x}$ where Δ means 'the difference'. Similarly when we differentiate we are effectively drawing an infinitely small triangle to calculate the rate of change (or gradient). This might seem quite an abstract concept and a full explanation lies beyond the scope of this booklet where we present the main properties of differentiation. When differentiate we use the notation:

$$\frac{dy}{dx}$$

where the d stands for an infinitely small difference. (We don't use Δ anymore as this represents a larger, not infinitely small, difference).

Example:

The derivative of x^2, as you will soon learn, is $2x$. Using the notation above we would write this as:

$$\text{If } y = x^2 \text{ then } \frac{dy}{dx} = 2x$$

Recall how we can write either y or $f(x)$ this leads to other notation for differentiation displayed in the table below:

Function	Derivative	Pronunciation
y	$\frac{dy}{dx}$	'd-y by d-x' **or** 'd-y d-x'
$f(x)$	$f'(x)$	'f prime of x' **or** 'f dash of x'
$f(x)$	$\frac{d}{dx}(f(x))$	'd by d-x of f of x'

Note: We may sometimes refer to $\frac{d}{dx}$ as the differential operator.

Example:

So if $f(x) = x^2$ then we can write the derivative in the following ways:

$$f'(x) = 2x$$

OR

$$\frac{d}{dx}(x^2) = 2x$$

IMPORTANT: When we find $\frac{dy}{dx}$ we said we are 'differentiating y with respect to x'. Now suppose instead that we have the equation $\theta = t^2$ then:

$$\frac{d\theta}{dt} = 2t$$

This works in the same way as we have seen for x and y but in this case we have it in terms of θ and t and would say we are 'differentiating θ with respect to t'.

4.2 Differentiating Polynomials

A polynomial is an equation in the form

$$a_nx^n + a_{n-1}x^{n-1} + \cdots + a_2x^2 + a_1x + a_0$$

where

- $a_n, \ldots, a_2, a_1, a_0$ are constant coefficients.
- $x^n, x^{n-1}, \ldots, x^2$ are powers of a variable x.

A rather simple example of a polynomial is the quadratic $x^2 + 3x + 1$.

Differentiation finds the gradient of a curve at a given point. Suppose we want to find the gradient of a function that is a polynomial such as $y = x^3 + 1$ how do we find this differential?

As differentiation may be new to many readers we will begin slowly and first explain how to differentiate the individual terms of a polynomial for example x^2 before moving on in the section on 'how to differentiate a sum' to help us differentiate polynomial sums such as $4x^3 + 1$.

The general rule is as follows:

$$\boxed{\text{If } y = x^n \text{ then } \frac{dy}{dx} = nx^{n-1}}$$

The main points we should note are that:

- If $y = 1$ then $\frac{dy}{dx} = 0$ (since $x^0 = 1$, so $n = 0$ here). In fact the same can be applied to any constant not just 1. So:

$$\boxed{\text{If } y = c \text{ for any constant } c \text{ then } \frac{dx}{dy} = 0.}$$

- If we have $y = x$ then this is the same as $y = x^1$ so we have $\frac{dy}{dx} = 1 \times x^{1-1} = 1$.
- If we have $y = x^2$ then we have $\frac{dy}{dx} = 2 \times x^{2-1} = 2x$.

We have only considered examples of polynomials up to the power of 2. The next example shows that we can apply this rule to polynomials of higher powers.

Example: Differentiate $y = x^5$.

Solution: From above we know if $y = x^n$ then $\frac{dy}{dx} = nx^{n-1}$. So in this example we have that $n = 5$. This gives the following answer:

$$\frac{dy}{dx} = 5x^{5-1} = 5x^4$$

We can also differentiate using this rule when x is raised to a negative power as shown in the next example.

Example: Differentiate $y = x^{-1}$.

Solution: From above we know if $y = x^n$ then $\frac{dy}{dx} = nx^{n-1}$. So in this example we have that $n = -1$. This gives the following answer:

$$\frac{dy}{dx} = -1 \times x^{-1-1} = -x^{-2}$$

We can differentiate using this rule when x is raised to a fractional power as shown in the next example.

Example: Differentiate $y = x^{\frac{1}{2}}$.

Solution: So using the rule if $y = x^n$ then $\dfrac{dy}{dx} = nx^{n-1}$ we have $n = \dfrac{1}{2}$. This gives the answer:

$$\frac{dy}{dx} = \frac{1}{2} \times x^{\frac{1}{2}-1} = \frac{x^{-\frac{1}{2}}}{2}$$

So far we have only considered polynomials which have a coefficient of 1. But how do we differentiate $y = 4x^2$ where the coefficient is equal to 4? When we have a coefficient denoted a we have the rule:

$$\boxed{\text{If } y = ax^n \text{ then } \frac{dy}{dx} = a \times n \times x^{n-1}}$$

Note: The first rule is just a special case of the above rule when $a = 1$.

So going back to $y = 4x^2$ we can see that the coefficient $a = 4$ and x is raised to the power of $n = 2$. So using the rule if $y = ax^n$ then $\dfrac{dy}{dx} = a \times n \times x^{n-1}$. We have:

$$\frac{dy}{dx} = 4 \times 2 \times x^{2-1} = 8x^1 = 8x$$

IMPORTANT: When differentiating any function $f(x)$ multiplied by some constant a, finding $\frac{d}{dx}[af(x)]$, we can take the constant a out of the derivative so:

$$\boxed{\frac{d}{dx}[af(x)] = a\frac{d}{dx}[f(x)]}$$

For example $\dfrac{d}{dx}(2x^3) = 2 \times \dfrac{d}{dx}(x^3) = 2 \times 3x^2 = 6x^2$.

Example: Differentiate $y = 4x^{-\frac{1}{2}}$

Solution: This example combines everything we have looked at so far. So using the rule:

$$\text{If } y = ax^n \text{ then } \frac{dy}{dx} = a \times n \times x^{n-1}$$

we have $a = 4$ and $n = -\dfrac{1}{2}$. This gives the answer:

$$\frac{dy}{dx} = 4 \times -\frac{1}{2} \times x^{-\frac{1}{2}-1} = -2x^{-\frac{3}{2}}$$

Chemistry Example: Coulomb's Law states that the magnitude of the attractive force ϕ between two charges decays according to the inverse square of the intervening distance r:

$$\phi = \frac{1}{r^2}$$

Suppose we plot a graph of ϕ on the y-axis against r on the x-axis what is the gradient?

Solution: To find the gradient we find the derivative with respect to r denoted $\dfrac{d\phi}{dr}$ of:

$$\phi = \frac{1}{r^2} = r^{-2}$$

All the examples so far have only contained x and y however in this question we have the variables ϕ and r. We know $y = x^n$ then $\dfrac{dy}{dx} = nx^{n-1}$ so with y as ϕ and x as r and $n = -2$. We have:

$$\frac{d\phi}{dr} = -2 \times r^{-2-1} = -2 \times r^{-3} = -\frac{2}{r^3}$$

4.3 Differentiating Trigonometric Functions

Below we have the rules for differentiating trigonometric functions:

$$\boxed{\text{If } y = \sin(x) \text{ then } \frac{dy}{dx} = \cos(x)}$$

$$\boxed{\text{If } y = \cos(x) \text{ then } \frac{dy}{dx} = -\sin(x)}$$

When we have constants multiplying the trigonometric functions and coefficients multiplying our x we can use the following rules:

$$\boxed{\text{If } y = a\sin(bx) \text{ then } \frac{dy}{dx} = a \times b \times \cos(bx)}$$

$$\boxed{\text{If } y = a\cos(bx) \text{ then } \frac{dy}{dx} = -a \times b \times \sin(bx)}$$

Note: These rules only work when x is being measured in radians.

Example: Differentiate:

1. $y = \sin(9x)$
2. $y = 4\cos\left(\frac{x}{2}\right)$
3. $y = -2\cos(-7x)$

Solution:

1. Using the rule:

$$\text{If } y = a\sin(bx) \text{ then } \frac{dy}{dx} = a \times b \times \cos(bx)$$

Note that we have $y = \sin(9x)$ so $a = 1$ and $b = 9$. So $\frac{dy}{dx} = 9\cos(9x)$

2. Using the rule:

$$\text{If } y = a\cos(bx) \text{ then } \frac{dy}{dx} = -a \times b \times \sin(bx)$$

Note that we have $y = 4\cos\left(\frac{x}{2}\right)$ so $a = 4$ and $b = \frac{1}{2}$

$$\frac{dy}{dx} = -4 \times \times \frac{1}{2} \times \sin\left(\frac{x}{2}\right) = -2\sin\left(\frac{x}{2}\right)$$

3. Using the rule:

$$\text{If } y = a\cos(bx) \text{ then } \frac{dy}{dx} = -a \times b \times \sin(bx)$$

Note that we have $y = -2\cos(-7x)$ so $a = -2$ and $b = -7$

$$\frac{dy}{dx} = -(-2) \times (-7\sin(-7x)) = -14\sin(-7x)$$

Chemistry Example: In X-ray crystallography, the Bragg equation relates the distance d between successive layers in a crystal, the wavelength of the X-rays λ, an integer n and the angle through which the X-rays are scattered θ in the equation:

$$\lambda = \frac{2d}{n}\sin\theta$$

What is the rate of change of λ with θ?

Solution: The question is asking us to find $\frac{d\lambda}{d\theta}$. So as n and d are constants we can use the rule:

$$\text{If } y = a\sin(bx) \text{ then } \frac{dy}{dx} = a \times b \times \cos(bx)$$

So we have $a = \left(\frac{2d}{n}\right)$ and $b = 1$ with λ as y and θ as x therefore:

$$\frac{d\lambda}{d\theta} = \left(\frac{2d}{n}\right) \times 1 \times \cos\theta = \frac{2d}{n}\cos\theta.$$

4.4 Differentiating Exponential and Logarithmic Functions

Differentiating Exponentials

The exponential function e^x when differentiated gives itself. This is shown is rule below:

$$\boxed{\text{If } y = e^x \text{ then } \frac{dy}{dx} = e^x}$$

We can also differentiate when the x has a coefficient for example $y = e^{4x}$ and also when the exponential is multiplied by a constant for example $y = 3e^x$. We combine these into the rule below:

$$\boxed{\text{If } y = ae^{bx} \text{ then } \frac{dy}{dx} = a \times b \times e^{bx}}$$

Example: Differentiate the following with respect to x:

1. $y = e^{2x}$
2. $y = 8\exp\left(-\frac{x}{3}\right)$

Solution:

1. Using the rule
$$\text{If } y = ae^{bx} \text{ then } \frac{dy}{dx} = a \times b \times e^{bx}$$
note $y = e^{2x}$ so $a = 1$ and $b = 1$ hence $\frac{dy}{dx} = 2e^{2x}$
2. Using the rule
$$\text{If } y = ae^{bx} \text{ then } \frac{dy}{dx} = a \times b \times e^{bx}$$
note $y = 8\exp\left(-\frac{x}{3}\right)$ so $a = 8$ and $b = -\frac{1}{3}$ hence $\frac{dy}{dx} = 8 \times -\frac{1}{3} \times \exp\left(-\frac{x}{3}\right) = -\frac{8}{3}e^{-\frac{x}{3}}$

Differentiating Logarithms

We differentiate logarithmic functions using the rule shown below:

$$\boxed{\text{If } y = \ln(x) \text{ then } \frac{dy}{dx} = \frac{1}{x}}$$

We can differentiate when the x has a coefficient for example $y = \ln(4x)$ and also when the logarithmic function has a coefficient for example $y = 3\ln(x)$. We combine these into the rules below:

$$\boxed{\text{If } y = a\ln(bx) \text{ then } \frac{dy}{dx} = \frac{a}{x}}$$

Note: In the above rule the b disappears and it forms a nice exercise in the practice of using the laws of logarithms hence we have included the algebra in the next example. We do have to differentiate a sum however so if you are unsure on that step then check out the next section for more help.

Example: For $y = a\ln(bx)$ find $\dfrac{dy}{dx}$

Solution: Using laws of logarithms we can write $y = a\ln(bx)$ as:

$$y = a\left(\ln(x) + \ln(b)\right)$$

Now differentiating this as a sum gives:

$$\frac{dy}{dx} = \frac{d}{dx}\left[a(\ln(x) + \ln(b))\right]$$
$$\implies \frac{dy}{dx} = a\frac{d}{dx}\left[\ln(x)\right] + a\frac{d}{dx}\left[\ln(b)\right]$$

Now as $\dfrac{d}{dx}\left[\ln(x)\right] = \dfrac{1}{x}$ and $\dfrac{d}{dx}\left[\ln(b)\right] = 0$ as $\ln(b)$ is a constant, so we have:

$$\frac{dy}{dx} = \frac{a}{x}$$

Note: The above derivation is included as it provides an advanced example of the use of the laws of logarithms with differentiation.

Example: Differentiate:

1. $y = \ln(3x)$
2. $y = -\dfrac{4}{5}\ln\left(\dfrac{x}{2}\right)$

Solution:

1. We use the rule:

   $$\text{If } y = a\ln(bx) \text{ then } \frac{dy}{dx} = \frac{a}{x}$$

   Note that we have $y = \ln(3x)$ so $a = 1$ and $b = 3$. Hence $\dfrac{dy}{dx} = \dfrac{1}{x}$

2. We use the rule:

   $$\text{If } y = a\ln(bx) \text{ then } \frac{dy}{dx} = \frac{a}{x}$$

   Note that we have $y = -\dfrac{4}{5}\ln\left(\dfrac{x}{2}\right)$ so $a = -\dfrac{4}{5}$ and $b = \dfrac{1}{2}$. Hence $\dfrac{dy}{dx} = -\dfrac{4}{5} \times \dfrac{1}{x} = -\dfrac{4}{5x}$

4.5 Differentiating a Sum

If we have multiple terms in the form of a sum for example $y = x^3 + 8x + 1$ then in order to find $\frac{dy}{dx}$ we apply the differential operator on each of the terms in turn. So in other words we differentiate each part of the sum one by one.

Consider $y = x^3 + 8x + 1$. If we want to find $\frac{dy}{dx}$ then we would apply the operator $\frac{d}{dx}$ to both sides of the equation giving us:

$$
\begin{aligned}
\frac{dy}{dx} &= \frac{d}{dx}(x^3 + 8x + 1) && \text{Now we apply the } \frac{d}{dx} \text{ operator to each term.}\\
\Longrightarrow \frac{dy}{dx} &= \frac{d}{dx}(x^3) + \frac{d}{dx}(8x) + \frac{d}{dx}(1) && \text{Now we differentiate each of the terms individually.}\\
\Longrightarrow \frac{dy}{dx} &= 3x^2 + 8x + 0 && \text{Now simplify.}\\
\Longrightarrow \frac{dy}{dx} &= 3x^2 + 8x
\end{aligned}
$$

Example: Differentiate the following:

1. $y = e^x + 4x^6$
2. $y = \ln(2x) + \frac{1}{3}\sin(9x)$

Solution:

1. To differentiate y we differentiate all of the terms individually. We use the rules for differentiating exponentials and powers to get:

$$y = e^x + 4x^6 \Longrightarrow \frac{dy}{dx} = e^x + 4 \times 6x^5 = e^x + 24x^5$$

2. Same as the example before we differentiate each term.

$$y = \ln(2x) + \frac{1}{3}\sin(9x) \Longrightarrow \frac{dy}{dx} = \frac{1}{x} + \frac{1}{3} \times 9\cos(9x) = \frac{1}{x} + 3\cos(9x)$$

Example: Differentiate $z = \cos(4t) + 6e^t + t^5 + 2t^2 + 7$ with respect to t.

Solution: This question is different as our equation is not in terms of y and x, but instead in terms of z and t. We treat this in the same way as if the terms were y and x so we differentiate each term individually.

$$\frac{dz}{dt} = -4\sin(4t) + 6e^t + 5t^4 + 4t$$

Example: The Onsager equation $\Lambda = \Lambda^o - b\sqrt{c}$ describes the relationship between the conductivity Λ of a simple ionic salt in solution and the concentration c where the limiting conductivity Λ^o and b are constants. Find $\frac{d\Lambda}{dc}$

Solution: As with the previous example, we aren't using x and y. we can write $\sqrt{c}$ as the fractional power $c^{\frac{1}{2}}$. This gives us $\Lambda = \Lambda^o - bc^{\frac{1}{2}}$. We can then differentiate this with respect to c.

$$
\begin{aligned}
\frac{d\Lambda}{dc} &= \frac{d}{dc}(\Lambda^o) - b\frac{d}{dc}\left(c^{\frac{1}{2}}\right) && \text{We can now differentiate each of the terms}\\
\frac{d\Lambda}{dc} &= 0 - b\left(\frac{1}{2}c^{-\frac{1}{2}}\right) && \text{Then expand and simplify}\\
\frac{d\Lambda}{dc} &= -\frac{b}{2}c^{-\frac{1}{2}}
\end{aligned}
$$

4.6 Product Rule

Suppose we want to differentiate $y = x^2\sin(x)$ then we encounter the problem: How to differentiate a function that is the product of two other functions, in this case x^2 and $\sin(x)$.

Do do this we need the product rule:

If the function $y = f(x)$ is written as the product of two functions say $u(x)$ and $v(x)$ so

$$y = f(x) = u(x)v(x) \;\; \text{then} \;\; \frac{dy}{dx} = u\frac{dv}{dx} + v\frac{du}{dx}$$

So returning to our example we have $f(x) = x^2\sin(x)$ with $u = x^2$ and $v = \sin(x)$.

First we find that $\dfrac{du}{dx} = 2x$ and $\dfrac{dv}{dx} = \cos(x)$ then we substitute into $\dfrac{dy}{dx} = u\dfrac{dv}{dx} + v\dfrac{du}{dx}$

$$\implies \frac{dy}{dx} = x^2\cos(x) + \sin(x)2x$$

$$\implies \frac{dy}{dx} = x(x\cos(x) + 2\sin(x))$$

Example: Differentiate using the product rule:

1. $y = x\ln(x)$

   Click here for a video example

2. $y = 6e^x\cos(x)$

   Click here for a video example

Solution:

1. Take $u = x$ and $v = \ln(x)$.
   We can now differentiate these to find that $\dfrac{du}{dx} = 1$ and that $\dfrac{dv}{dx} = \dfrac{1}{x}$

   Using the product rule:

$$\begin{aligned} \frac{dy}{dx} &= u\frac{dv}{dx} + v\frac{du}{dx} && \text{Substitute in the quantities} \\ \frac{dy}{dx} &= x\left(\frac{1}{x}\right) + \ln(x)\Big(1\Big) && \text{Expand and simply} \\ \frac{dy}{dx} &= 1 + \ln(x) \end{aligned}$$

2. For this take $u = 6e^x$ and $v = \cos(x)$.
   Now we differentiate those find that $\dfrac{du}{dx} = 6e^x$ and $\dfrac{dv}{dx} = -\sin(x)$

   By the product rule we have:

$$\begin{aligned} \frac{dy}{dx} &= u\frac{dv}{dx} + v\frac{du}{dx} && \text{Substitute in the quantities} \\ \frac{dy}{dx} &= 6e^x\Big(-\sin(x)\Big) + \cos(x)\Big(6e^x\Big) && \text{Expand the brackets} \\ \frac{dy}{dx} &= -6e^x\sin(x) + 6e^x\cos(x) && \text{Take a factor of } 6e^x \text{ out} \\ \frac{dy}{dx} &= 6e^x\Big(\cos(x) - \sin(x)\Big) \end{aligned}$$

Example: Differentiate $y = \frac{1}{3}(x^2 + 5x)\sin(x)$.

Solution: This is a product of two function and we must use the product rule.

Set $u = \frac{1}{3}(x^2 + 5x)$ and $v = \sin(x)$

We can differentiate to find that $\frac{du}{dx} = \frac{1}{3}(2x + 5)$ and $\frac{dv}{dx} = \cos(x)$

We now use the product rule:

$$\frac{dy}{dx} = u\frac{dv}{dx} + v\frac{du}{dx} \qquad \text{Substitute in what we've worked out}$$

$$\frac{dy}{dx} = \frac{1}{3}(x^2 + 5x)\Big(\cos(x)\Big) + \sin(x)\Big(\frac{1}{3}(2x + 5)\Big) \qquad \text{Simplify by taking a factor of } \frac{1}{3} \text{ out}$$

$$\frac{dy}{dx} = \frac{1}{3}\Big((x^2 + 5x)\cos(x) + (2x + 5)\sin(x)\Big)$$

The end result looks complicated and ugly but it is nicer than having all the brackets expanded.

4.7 Quotient Rule

A quotient looks like a fraction with one function being divided by another function for example:

$$y = \frac{x^3}{e^{3x}}$$

When we have a function in the form of a quotient we differentiate it using the quotient rule:

If the function $f(x)$ is written as a quotient so

$$y = \frac{u(x)}{v(x)} \quad \text{then} \quad \frac{dy}{dx} = \frac{v\frac{du}{dx} - u\frac{dv}{dx}}{v^2}$$

So returning to $y = \dfrac{x^3}{e^{3x}}$ we have $u = x^3$ and $v = e^{3x}$.

Hence $\dfrac{du}{dx} = 3x^2$ and $\dfrac{dv}{dx} = 3e^{3x}$ and $v^2 = e^{6x}$. Then substitute into quotient rule $\dfrac{dy}{dx} = \dfrac{v\frac{du}{dx} - u\frac{dv}{dx}}{v^2}$

$$\implies \frac{dy}{dx} = \frac{e^{3x}3x^2 - x^3 3e^{3x}}{e^{6x}}$$

$$\implies \frac{dy}{dx} = 3x^2 e^{-3x}(1 - x)$$

Example: Differentiate $y = \dfrac{\sin(x)}{3\ln(x)}$.

Solution: Just like the previous example we have u to be the numerator and v to be the denominator of the fraction so $u = \sin(x)$ and $v = 3\ln(x)$. We can now differentiated these to get $\dfrac{du}{dx} = \cos(x)$ and $\dfrac{dv}{dx} = \dfrac{3}{x}$. Using the quotient rule we get that:

$$\frac{dy}{dx} = \frac{v\frac{du}{dx} - u\frac{dv}{dx}}{v^2} \qquad \text{Substitute in what we have}$$

$$\frac{dy}{dx} = \frac{3\ln(x) \times \cos(x) \ - \ \sin(x) \times \frac{3}{x}}{\left(3\ln(x)\right)^2} \qquad \text{We can simplify}$$

$$\frac{dy}{dx} = \frac{3\ln(x)\cos(x) \ - \ \frac{3\sin(x)}{x}}{9\ln(x)^2} \qquad \text{A factor of 3 can be taken out}$$

$$\frac{dy}{dx} = \frac{\ln(x)\cos(x) \ - \ \frac{\sin(x)}{x}}{3\ln(x)^2}$$

Example: Differentiate $y = \frac{x}{e^{2x}}$

Click here for a video example

Solution: We have a function x divided by a function e^{2x} so to find the derivative the quotient rule needs to be used. So $u = x$ and $v = e^{2x}$ and therefore $\frac{du}{dx} = 1$ and $\frac{dv}{dx} = 2e^{2x}$. We can now employ the quotient rule to get:

$$\frac{dy}{dx} = \frac{v\frac{du}{dx} - u\frac{dv}{dx}}{v^2} \qquad \text{Substitute what we know in}$$

$$\frac{dy}{dx} = \frac{e^{2x} \times 1 - x \times 2e^{2x}}{(e^{2x})^2} \qquad \text{Simplifying this by taking a factor of } e^{2x} \text{ out}$$

$$\frac{dy}{dx} = \frac{e^{2x}(1-2x)}{(e^{2x})^2} \qquad \text{The } e^{2x} \text{ on top cancels with one on the bottom}$$

$$\frac{dy}{dx} = e^{-2x}(1-2x)$$

Chemistry Example: During the reaction $N_2O_4 \rightleftharpoons 2\,NO_2$ the partial pressure of N_2O_4 is given by the expression $p_{(N_2O_4)} = \frac{1-\zeta}{1+\zeta}$. Find $\frac{dp}{d\zeta}$.

Solution: We notice that p is the quotient of two functions involving ζ this means that we should use the quotient rule when differentiating. So we have $u = 1-\zeta$ and $v = 1+\zeta$. Differentiating gives us $\frac{du}{d\zeta} = -1$ and $\frac{dv}{d\zeta} = 1$. We then utilise the quotient rule to find that:

$$\frac{dp}{d\zeta} = \frac{v\frac{du}{d\zeta} - u\frac{dv}{d\zeta}}{v^2} \qquad \text{So we first substitute.}$$

$$\frac{dp}{d\zeta} = \frac{(1+\zeta) \times (-1) \ - \ (1-\zeta) \times 1}{(1+\zeta)^2} \qquad \text{Expand the brackets.}$$

$$\frac{dp}{d\zeta} = \frac{-1-\zeta \ - \ 1+\zeta}{(1+\zeta)^2} \qquad \text{Simplifying the numerator.}$$

$$\frac{dp}{d\zeta} = \frac{-2}{(1+\zeta)^2}$$

4.8 Chain Rule

When we have one function inside another function (this is called a composite function) we differentiate using the chain rule. An example of a composite function is $y = \sin(x^2 + 1)$. There are two functions $\sin(..)$ and $x^2 + 1$. We are applying the sin function to $x^2 + 1$, thus making it a function inside a function or a composite function.

The general form of a composite function is:

$$\boxed{y = f(g(x))}$$

where f and g are both functions. In the above example $y = \sin(x^2+1)$ we would have $f(g(x)) = \sin(g(x))$ and $g(x) = x^2 + 1$.

$$y = \sin(\underbrace{x^2 + 1})$$

Outer function, $f(..)$ Inner function, $g(x)$

To use the chain rule we use the following steps:

1. Introduce a new variable u to be equal to $u = g(x)$.
2. Substitute $u = g(x)$ into the expression $y = f(g(x))$ so that $y = f(u)$.
3. Find $\dfrac{dy}{du}$ and $\dfrac{du}{dx}$.
4. The derivative $\dfrac{dy}{dx}$ can be found by this equation $\dfrac{dy}{dx} = \dfrac{dy}{du} \times \dfrac{du}{dx}$ and then substitute back in $u = g(x)$.

The chain rule is summarised in the box below:

$$\boxed{\begin{array}{c} \text{If } y = f(g(x)) \quad \text{let} \quad u = g(x) \quad \text{hence} \quad y = f(g(x)) = f(u) \\ \text{then} \quad \dfrac{dy}{dx} = \dfrac{dy}{du} \times \dfrac{du}{dx} \end{array}}$$

Below we follow the steps of the chain rule to differentiate $y = \sin(x^2 + 1)$:

1. Introduce a new variable u to be equal to $g(x)$ (the inside function). For this example $u = x^2 + 1$.
2. Substitute $u = g(x)$ into the expression $y = f(g(x))$ so that $y = f(u)$. As $u = x^2 + 1$ this would make $y = \sin(u)$.
3. Find $\dfrac{dy}{du}$ and $\dfrac{du}{dx}$. In this example we have:

$$y = \sin(u) \Longrightarrow \frac{dy}{du} = \cos(u)$$

and

$$u = x^2 + 1 \Longrightarrow \frac{du}{dx} = 2x$$

4. The derivative $\dfrac{dy}{dx}$ can be found by this equation $\dfrac{dy}{dx} = \dfrac{dy}{du} \times \dfrac{du}{dx}$ and then substitute back in $u = g(x)$.

$$\Longrightarrow \frac{dy}{dx} = \cos(u) \times 2x = 2x\cos(x^2 + 1)$$

Example: Differentiate $y = (x^2+2)^3$ using the chain rule:

Click here for a video example

Solution: We take $u = x^2 + 2$ and therefore $y = u^3$.

Then we differentiate each of those to find:

$$\frac{du}{dx} = 2x \qquad \frac{dy}{du} = 3u^2$$

From the chain rule:

$$\begin{aligned}
\frac{dy}{dx} &= \frac{dy}{du} \times \frac{du}{dx} && \text{Substitute in what we know for } \frac{dy}{du} \text{ and } \frac{du}{dx} \\
\frac{dy}{dx} &= 3u^2 \times 2x && \text{Substitute that } u \text{ is } x^2+2 \\
\frac{dy}{dx} &= 6x(x^2+2)^2
\end{aligned}$$

Example: Given $y = \ln(x^3)$ find $\frac{dy}{dx}$

Click here for a video example

Solution: We take $u = x^3$ which means that $y = \ln(u)$.

Then differentiate to find that:

$$\frac{du}{dx} = 3x^2 \qquad \frac{dy}{du} = \frac{1}{u}$$

From the chain rule $\frac{dy}{dx} = \frac{dy}{du} \times \frac{du}{dx}$ we can see that:

$$\begin{aligned}
\frac{dy}{dx} &= \frac{1}{u} \times 3x^2 && \text{Substitute that } u \text{ is } x^3 \\
\frac{dy}{dx} &= \frac{1}{x^3} \times 3x^2 && \text{Simplify further} \\
\frac{dy}{dx} &= \frac{3}{x}
\end{aligned}$$

Note: A faster solution would have been to use the laws of logarithms to notice that $\ln(x^3) = 3\ln(x)$ and then differentiate avoiding the use of the chain rule.

Example: Differentiate $y = \cos(e^{2x})$

Solution: Let $u = e^{2x}$ therefore $y = \cos(u)$.

Differentiate to find:

$$\frac{du}{dx} = 2e^{2x} \text{ and } \frac{dy}{du} = -\sin(u)$$

Using the chain rule $\frac{dy}{dx} = \frac{dy}{du} \times \frac{du}{dx}$ we can show that:

$$\begin{aligned}
\frac{dy}{dx} &= -\sin(u) \times 2e^{2x} && \text{Substitute that } u = e^{2x} \\
\frac{dy}{dx} &= -2e^{2x}\sin(e^{2x})
\end{aligned}$$

Chemistry Example: The Maxwell Boltzmann Distribution is a probability distribution of finding particles at certain speed v in 3 dimensions. It has the form of:

$$f(v) = Av^2 e^{-Bv^2}$$

where A and B are positive constants. Using the chain rule and the product rule find $\frac{d}{dv}f(v)$.

Solution: This example involves two steps, first of all the product rule is required to differentiate whole thing as $f(v)$ is a product of two functions. The chain rule is also needed to differentiate the exponential. Lets call $P = Av^2$ and $Q = e^{-Bv^2}$, thus making $f(v) = P \times Q$. From the product rule:

$$\frac{d}{dv}f(v) = P\frac{dQ}{dv} + Q\frac{dP}{dv}$$

We have $\frac{dP}{dv} = 2Av$ but we will need to use the chain rule to find $\frac{dQ}{dv}$.

We let $u = -Bv^2$, making $Q = e^u$. We can then calcuate that $\frac{du}{dv} = -2Bv$ and that $\frac{dQ}{du} = e^u$. From here the chain rule tells us that:

$$\frac{dQ}{dv} = \frac{dQ}{du} \times \frac{du}{dv} \qquad \text{We put in what we have for } \frac{dQ}{du} \text{ and } \frac{du}{dv}$$

$$\frac{dQ}{dv} = e^u \times (-2Bv) \qquad \text{Substitute } u = -Bv^2$$

$$\frac{dQ}{dv} = -2Bv \cdot e^{-Bv^2}$$

Substituting into the previous equation (shown below) gives us:

$$\frac{d}{dv}f(v) = P\frac{dQ}{dv} + Q\frac{dP}{dv} \qquad \text{Substitute in what we have found}$$

$$\frac{d}{dv}f(v) = Av^2(-2Bv \times e^{-Bv^2}) + e^{-Bv^2} \times 2Av \qquad \text{This can be simplified}$$

$$\frac{d}{dv}f(v) = -2ABv^3 e^{-Bv^2} + 2Av\, e^{-Bv^2} \qquad \text{Take a factor of } 2Av\, e^{-Bv^2} \text{ out}$$

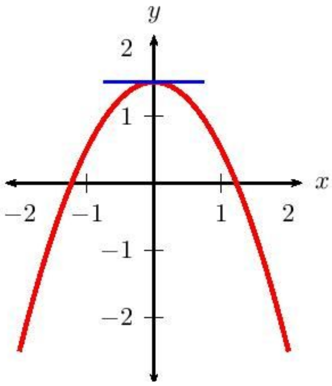
$$\frac{d}{dv}f(v) = 2Av\, e^{-Bv^2}(1 - Bv^2)$$

Note: This example is complex since we are using multiple rules. Not all problems will be this hard, but it's important to know how to combine the rules of differentiation. An application of this derivative would be to find the modal speed of a gas.

4.9 Stationary Points

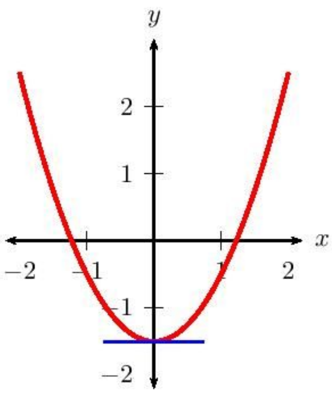
Stationary points occur when we have $\frac{dy}{dx} = 0$; this represents when the gradient of a curve is horizontal we have three type of stationary points:

1. Local maximum



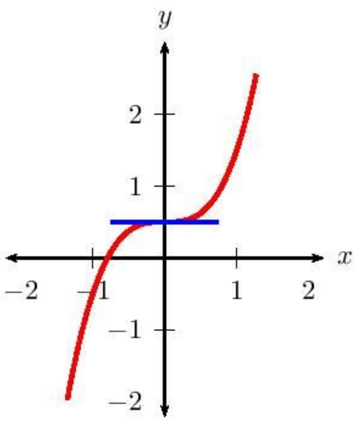
   We can see that when we pass through a maximum at the gradient goes from being positive ($f'(x) > 0$ or $\frac{dy}{dx} > 0$) to being negative ($f'(x) < 0$ or $\frac{dy}{dx} < 0$).

2. Local minimum



   We can see that when we pass through a minimum the gradient goes from being negative i.e. $f'(x) < 0$ (or $\frac{dy}{dx} < 0$) to being positive i.e. $f'(x) > 0$ (or $\frac{dy}{dx} > 0$).

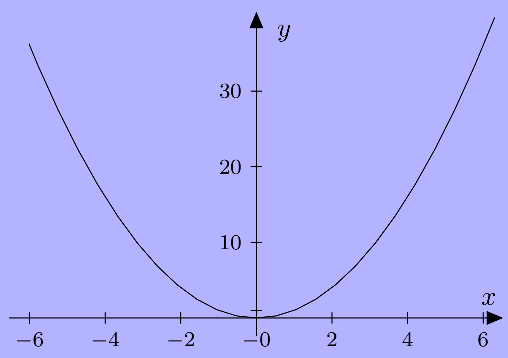
3. Point of inflection



   Finally when we pass through point of inflection we should note that the gradient remains of the same sign (so either positive both sides or negative both sides).

Example: Find the stationary point of $y = x^2$

Solution: From the graph of $y = x^2$ we can see that there is a minimum at $x = 0$ however we need to find this algebraically.



First we need to find when $\frac{dy}{dx} = 0$. Now $\frac{dy}{dx} = 2x$ and therefore $\frac{dy}{dx} = 0$ when $x = 0$.

So we know we have a stationary point at $x = 0$ in the next section we will discuss how to decide whether this is a maximum, minimum or point of inflection.

Classifying Stationary Points

We now need to introduce the second derivative denoted:

$$\frac{d^2y}{dx^2} \quad \text{or} \quad f''(x)$$

This means that we differentiate a function twice so for example if we have $y = x^3$ we would first find:

$$\frac{dy}{dx} = 3x^2$$

which we would then differentiate again to find:

$$\frac{d^2y}{dx^2} = 6x$$

First Test

The second derivative is used to decide whether a stationary point is a maximum or a minimum. If we have the value of x of a stationary point then we substitute this value into the second derivative, if:

- $\frac{d^2y}{dx^2} > 0$ so positive we have a minimum.
- $\frac{d^2y}{dx^2} < 0$ so negative we have a maximum.

Unfortunately this test fails if we find that $\frac{d^2y}{dx^2} = 0$. In this case we could have a maximum, minimum or point of inflection and we must carry out the following further test in order to decide:

Second Test

First find two x values just to the left and right of the stationary point and calculate $f'(x)$ for each. Let use denote the x value just to the left as x_L and the one to the right as x_R then if:

- $f'(x_L) > 0$ and $f'(x_R) < 0$ we have a maximum.
- $f'(x_L) < 0$ and $f'(x_R) > 0$ we have a minimum.
- $f'(x_L)$ and $f'(x_R)$ have the same sign (so both are either positive or negative) then we have a point of inflection.

Example: Find and classify the stationary points of $y = \frac{x^4}{4} - \frac{x^2}{2}$

Click here for a video example

Solution: First we find when $\frac{dy}{dx} = 0$ to find where the stationary points are.

$$\frac{dy}{dx} = x^3 - x = 0$$
$$\implies x(x^2 - 1) = 0$$
$$\implies x(x-1)(x+1) = 0$$

Therefore we have stationary points at $x = 0$, $x = 1$ and $x = -1$ to classify them we first must find the second derivative:

$$\frac{d^2y}{dx^2} = 3x^2 - 1$$

Now we substitute our x-values for the location of the stationary point into $\frac{d^2y}{dx^2}$.

- Now when $x = 0$ we have $\frac{d^2y}{dx^2} = -1$ hence $\frac{d^2y}{dx^2} < 0$ (negative) so this is a maximum.
- Now when $x = 1$ we have $\frac{d^2y}{dx^2} = 2$ hence $\frac{d^2y}{dx^2} > 0$ (positive) so this is a minimum.
- Now when $x = -1$ we again have $\frac{d^2y}{dx^2} = 2$ hence $\frac{d^2y}{dx^2} > 0$ (positive) so this is a minimum.

Example: Find and classify the stationary points of $y = x^3$

Solution: First we find when $\frac{dy}{dx} = 0$ to find where the stationary points are.

$$\frac{dy}{dx} = 3x^2 = 0$$
$$\implies x = 0$$

Therefore we have one stationary point at $x = 0$. To classify this point we need to find the second derivative:

$$\frac{d^2y}{dx^2} = 6x$$

Now when $x = 0$ we have $\frac{d^2y}{dx^2} = 0$ hence our test has failed and we must carry out the further test.

Now we need to pick x values close to either side of the stationary point at $x = 0$. So a x value just to the left would be $x_L = -0.5$ and one just to the right would be $x_R = 0.5$.

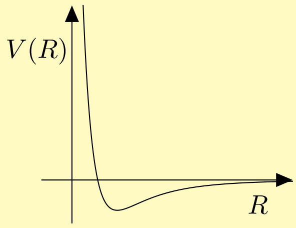
Now as $\frac{dy}{dx} = f'(x) = 3x^2$ we have that:

- $f'(x_L) = 3(x_L)^2 = 3 \times -0.5^2 = 0.75 > 0$
- $f'(x_R) = 3(x_R)^2 = 3 \times 0.5^2 = 0.75 > 0$

So both $f'(x_L) > 0$ and $f'(x_R) > 0$ are positive so are of the same sign. Hence the stationary point at $x = 0$ is a point of inflection.

Chemistry Example: The Lennard-Jones potential decribes the potential energy V between two helium atoms separated by a distance R. The equation and graph of this function are shown below:

$$V(R) = \frac{A}{R^{12}} - \frac{B}{R^6}$$



where A and B are constants. The two particles are at their equilibrium separation when the potential is at a minimum (V is at a minimum). By differentiating this equation with respect to R find the equilibrium separation.

Click here for a video example

Solution: To find the minimum V we need to differentiate it and then set it equal to zero (find $\frac{dV}{dR} = 0$). Then that value of R will be where the potential is a minimum. Differentiating V with respect to R gives:

$$\frac{dV}{dR} = \frac{-12A}{R^{13}} + \frac{6B}{R^7}$$

We need to find when $\dfrac{dV}{dR} = 0$ so need to solve the equation:

$$\begin{aligned}
\frac{-12A}{R^{13}} + \frac{6B}{R^7} &= 0 && \text{Add } \frac{-12A}{R^{-13}} \text{ to both sides} \\
\frac{6B}{R^7} &= \frac{12A}{R^{13}} && \text{Multiply each side by } R^{13} \text{ and divide by } 6B \\
\frac{R^{13}}{R^7} &= \frac{12A}{6B} && \text{Simplify both of the fractions} \\
R^6 &= \frac{2A}{B} && \text{Take the 6th root of both sides} \\
R &= \left(\frac{2A}{B}\right)^{\frac{1}{6}}
\end{aligned}$$

Hence at the equilibrium separation $R = \left(\dfrac{2A}{B}\right)^{\frac{1}{6}}$.

4.10 Partial Differentiation

Often we encounter quantities that depend on more than one variable. For example the enthalpy H of a system depends on pressure P and temperature T. Another case is the ideal gas equation as seen below:

$$p = \frac{nRT}{V}$$

The pressure p of a gas depends on its volume V and the temperature T it is at. We often find it useful to calculate how one variable changes with one other while the remaining variables are seen to be constant.

Recall we can use the notation $y = f(x, z)$ to mean that y is a function of x and z where x and z are independent variables. For example:

$$y = x^2 + zx$$

We use partial derivatives to differentiate functions with multiple variables. We do this by differentiating with respect to one variable and treating all other variables as constants. So for $y = f(x, z)$ the partial derivative of a y with respect to x is denoted:

$$\left(\frac{\partial y}{\partial x}\right)_z$$

The curvy symbol ∂ informs us that we perform partial differentiation with respect to x while the subscript variable in this case z is being considered as a constant.

Note: Some books just use the notation $\dfrac{\partial y}{\partial x}$, taking it as understood that all other variables except x are taken as constant.

Example: So going back to our example $y = x^2 + zx$. Find $\left(\dfrac{\partial y}{\partial x}\right)_z$

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Solution: We note:

- The curvy symbol ∂ informs us that we perform partial differentiation.
- We are differentiating y with respect to x.
- We treat z as a constant.

So we differentiate the x^2 term as usual to get $2x$. Then we differentiate the zx term treating z as a constant so this gives z. Hence:

$$\left(\frac{\partial y}{\partial x}\right)_z = 2x + z$$

Example: For $y = 2\ln(z) + \sin(zx)$ find $\left(\dfrac{\partial y}{\partial x}\right)_z$ and $\left(\dfrac{\partial y}{\partial z}\right)_x$

Solution: For $\left(\dfrac{\partial y}{\partial x}\right)_z$ we treat z as a constant and differentiate with respect to x.

$$\left(\frac{\partial y}{\partial x}\right)_z = \frac{\partial}{\partial x} 2\ln(z) + \frac{\partial}{\partial x}\sin(zx) \qquad \text{Treating } z \text{ as a constant}$$

$$\left(\frac{\partial y}{\partial x}\right)_z = 0 + z\cos(zx) = z\cos(zx)$$

For $\left(\dfrac{\partial y}{\partial z}\right)_x$ we treat x like a constant and then differentiate with respect to z.

$$\left(\frac{\partial y}{\partial x}\right)_z = \frac{\partial}{\partial z} 2\ln(z) + \frac{\partial}{\partial z}\sin(zx) \qquad \text{Treating } x \text{ as a constant}$$

$$\left(\frac{\partial y}{\partial x}\right)_z = \frac{2}{z} + z\cos(zx)$$

Chemistry Example: The ideal gas equation is $pV = nRT$. Find:

1. $\left(\dfrac{\partial V}{\partial T}\right)_p$

2. $\left(\dfrac{\partial T}{\partial p}\right)_V$

Click here for a video example

Solution:

1. To be able to find $\left(\dfrac{\partial V}{\partial T}\right)_p$ we must first make V the subject in the equation. This is done by dividing both sides by p to produce $V = \dfrac{nRT}{p}$.

   Now we differentiate with respect to T taking p to be a constant.

$$\left(\frac{\partial V}{\partial T}\right)_p = \frac{\partial}{\partial T}\left(\frac{nRT}{p}\right) \quad \text{Note } \frac{nR}{p} \text{ is a constant.}$$

$$\left(\frac{\partial V}{\partial T}\right)_p = \frac{nR}{p}$$

   This is Charles's law, at constant pressure, the volume of a gas is directly proportional to the temperature.

2. We do the same process to find $\left(\dfrac{\partial T}{\partial p}\right)_V$. First make T the subject by dividing both sides by nR to make $T = \dfrac{PV}{nR}$.

   As before we then differentiate, treating V as a constant this time to get:

$$\left(\frac{\partial T}{\partial p}\right)_V = \frac{\partial}{\partial p}\left(\frac{pV}{nR}\right) \quad \text{Note } \frac{V}{nR} \text{ is a constant}$$

$$\left(\frac{\partial T}{\partial p}\right)_V = \frac{V}{nR}$$

   This is Gay-Lussac's (or the pressure) law: under fixed volume the pressure is proportional to the temperature.

5 Integration

5.1 Introduction to Integration

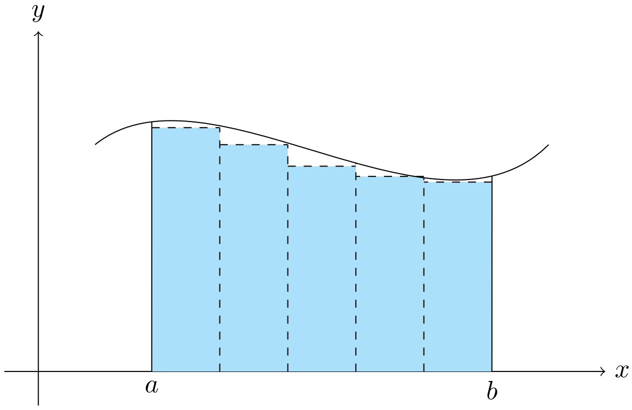
Integration is the opposite of differentiation so it helps us find the answer to the question:

$$\text{'Suppose we have } \frac{dy}{dx} = 2x \text{ then what is } y\text{?'}$$

From the previous section we know the answer is $x^2 + C$ where C is a constant. So we would say that $2x$ integrated is $x^2 + C$.

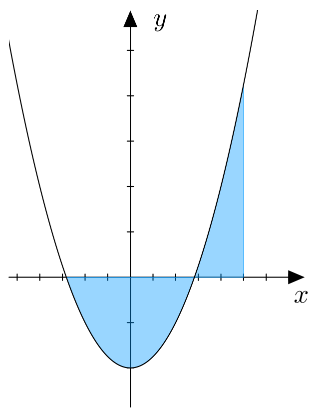
Note: We have an infinite number of solutions to above question as the constant C could be any number!

Graphically we know differentiation gives us the gradient of a curve. Integration finds the area beneath a curve.



Suppose we wish to find the area under the curve between the x values a and b shaded in the graph above. Then we could find an approximate answer by creating the dashed rectangles above and summing their area. Now we can see this does not give a perfect answer however the smaller the width of the rectangles the lower the error in our answer would be.

So if we could use rectangles of an infinitely small width we would find an answer with no error. This is what integration does. It creates an infinite number of rectangles under the curve all with an infinitely small width and sums their area to find the area under the curve.



So integration could be used to find the area shaded on the graph of $y = x^2 - 2$ above. Note that when the curve is below the x-axis integration finds the area bounded between the curve and the x-axis.

Note: If the area we are finding is below the x-axis then we get a negative answer when we integrate.

Notation

We use the fact that $2x$ integrated is $x^2 + C$ to help introduce the following notation for integration. If we want to integrate $2x$ we write this as:

$$\int 2x \, dx = x^2 + C$$

- The $\int$ tells us we need to integrate.
- The dx tells use to integrate with respect to x. So we could write $\int 2z \, dz = z^2 + C$ but in this case we have integrated with respect to z.
- We call $\int 2x \, dx = x^2 + C$ the integral.

Another notation often used is the following if we have the function $f(x)$ then we write this integrated as $F(x)$. So if $f(x) = 2x$ then $F(x) = x^2 + C$.

Integration finds the area under the curve. So if we want to find the area between two points (called limits) on the x-axis, say a and b, we use the following notation:

$$\int_a^b f(x) \, dx$$

This tell us we want to find the integral of $f(x)$ and then use that information to find the area under the curve between a and b. We find this area by using the formula below:

$$\boxed{\int_a^b f(x) \, dx = F(b) - F(a)}$$

Note: This is explained in detail in the section on definite integrals.

- When we are given limits the we have a definite integral.
- When we are not given limits the we have a indefinite integral.

Rules for Integrals

1. We can split integrals over a sum. For example $\int (x^3 + 2x + 7) \, dx = \int x^3 \, dx + \int 2x \, dx + \int 7 \, dx$.
2. We can take constants out of the integral. For example $\int 6x^4 \, dx = 6 \int x^4 \, dx$.

5.2 Integrating Polynomials

When we are differentiating x^n we multiply by n and then reduce the power on x by 1. When integrating we do the opposite first we add 1 to the power, then divide by this new power. In general we have the rule:

$$\boxed{\int x^n\,dx = \frac{x^{n+1}}{n+1} + C}$$

Note: This rule works for all values of n apart from $n = -1$. If we were to use the rule with $n = -1$ we would have $\frac{x^0}{0} + C$. This would have us dividing by 0 which is forbidden. The integral of x^{-1} is discussed on the next page.

Example: Find the integrals of the following:

1. x^2
2. $2x + 6x^2$
3. $x(x + 3)$

Solution:

1. We are being asked to find $\int x^2\,dx$ so using the rule $\int x^n\,dx = \dfrac{x^{n+1}}{n+1} + C$

$$\begin{aligned}\int x^2\,dx &= \frac{x^{2+1}}{2+1} + C && \text{This can be simplified}\\ &= \frac{x^3}{3} + C\end{aligned}$$

2. We are being asked to find $\int (2x + 6x^2)\,dx$.

When integrating multiple terms we do each of them one in turn. This means that:

$$\begin{aligned}\int (2x + 6x^2)\,dx &= \int 2x\,dx + \int 6x^2\,dx && \text{Constants are taken out of the integral}\\ &= 2\int x\,dx + 6\int x^2\,dx && \text{We can now integrate}\\ &= 2\,\frac{x^{1+1}}{1+1} + 6\,\frac{x^{2+1}}{2+1} + C && \text{This can be simplified}\\ &= x^2 + 2x^3 + C\end{aligned}$$

3. First we expand the brackets to produce $x^2 + 3x$. Then we would integrate this gives:

$$\begin{aligned}\int (x^2 + 3x)\,dx &= \frac{x^{2+1}}{2+1} + 3\frac{x^{1+1}}{1+1} + C && \text{This can be simplified}\\ &= \frac{1}{3}x^3 + \frac{3}{2}x^2 + C\end{aligned}$$

Integrating x^{-1}

We recall that if we differentiate $\ln(x)$ we get x^{-1}. Since integration is the opposite of differentiation, when we integrate x^{-1} we get $\ln(x)$.

$$\boxed{\int x^{-1}\,dx = \ln|x| + c}$$

Note: The $|$ signs either side of the x mean the modulus (or the absolute value) of x. It makes sure our x value is positive. For example $|5| = 5$ and $|-5| = 5$. It is important in this integral as we can input a negative value of x into x^{-1} however we cannot take the log of a negative x.

Example: Find the following integral:

$$\int \frac{x^2 + 2x^3 - 4x^4}{x^3}\,dx$$

Solution: The fraction can be simplified, by dividing each term on the denominator by x^3. This reduces the original integral into:

$$\begin{aligned}
\int \frac{x^2 + 2x^3 - 4x^4}{x^3}\,dx &= \int \left(\frac{1}{x} + 2 - 4x\right)dx && \text{Integrate each term individually}\\
&= \ln|x| + 2x + \frac{-4}{2}x^2 + C && \text{Simplify the terms}\\
&= \ln|x| + 2x - 2x^2 + C
\end{aligned}$$

5.3 Integrating Exponentials

We can recall that:

$$\boxed{\text{If } y = e^{ax} \text{ then } \frac{dy}{dx} = a \times e^{ax}}$$

So when we are differentiating e^{ax} we multiply the exponential by the coefficient of the power. When integrating we do the opposite so we divide by the coefficient of the power. In general we have:

$$\boxed{\int e^{ax}\,dx = \frac{e^{ax}}{a} + C}$$

Example: find the following:

1. $\displaystyle\int e^{6x}\,dx$
2. $\displaystyle\int (e^{x} + 4e^{-3x}\ )\,dx$
3. $\displaystyle\int 9e^{3z}\,dz$

Solution:

1. Using the rule $\displaystyle\int e^{ax}\,dx = \frac{e^{ax}}{a} + C$ and dividing by the coefficent of the power we find:
$$\int e^{6x}\,dx = \frac{e^{6x}}{6} + C$$
2. First we should break up the integral across the sum:
$$\int (e^{x} + 4e^{-3x})\,dx = \int e^{x}\,dx + 4\int e^{-3x}\,dx$$
Now we can apply the rule above to get:
$$\int e^{x}\,dx + 4\int e^{-3x}\,dx = \frac{e^{x}}{1} + 4 \times \frac{e^{-3x}}{-3} + C = e^{x} - \frac{4e^{-3x}}{3} + C$$
3. Using the rule above but this time with respect to z we find:
$$\int 9e^{3z}\,dz = 9\int e^{3z}\,dz = 9 \times \left(\frac{e^{3x}}{3} + C\right) = 3e^{3x} + C'$$
where $C' = 9C$.

5.4 Integrating Trigonometric Function

We can recall that:

$$\boxed{\text{If } y = \sin(ax) \text{ then } \frac{dy}{dx} = a\cos(ax)}$$

$$\boxed{\text{If } y = \cos(ax) \text{ then } \frac{dy}{dx} = -a\sin(ax)}$$

When integrating we do the opposite of differentiation so e:

$$\boxed{\int \cos(ax)\,dx = \frac{\sin(ax)}{a} + C}$$

$$\boxed{\int \sin(ax)\,dx = \frac{-\cos(ax)}{a} + C}$$

Example: find the following:

1. $\displaystyle\int \cos(4x)\,dx$

2. $\displaystyle\int 6\sin(3x)\,dx$

3. $\displaystyle\int \big(5\cos(-x) + \sin(3x)\big)\,dx$

Solution:

1. Using the rule $\displaystyle\int \cos(ax)\,dx = \frac{\sin(ax)}{a} + C$ a we find:

$$\int \cos(4x)\,dx = \frac{\sin(4x)}{4} + C$$

2. First we should note $\displaystyle\int 6\sin(3x)\,dx = 6\int \sin(3x)\,dx$

   Now we can apply the rules above to get:

$$\int 6\sin(3x)\,dx = 6\int \sin(3x)\,dx = 6 \times \frac{-\cos(3x)}{3} + C = -2\cos(3x)$$

3. Splitting up the integral and extracting constants gives:

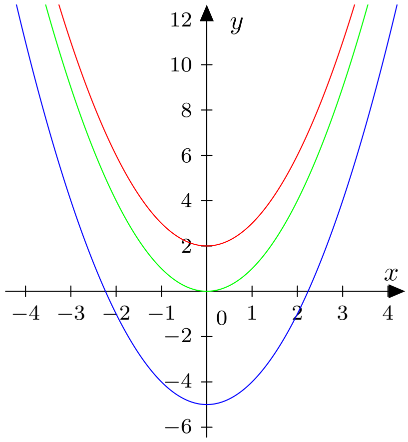
$$\int \big(5\cos(-x) + \sin(3x)\big)\,dx = 5\int \cos(-x)\,dx + \int \sin(3x)\,dx$$

   Now by applying the above rules we get:

$$\begin{aligned}\int 5\cos(-x) + \sin(3x)\,dx = \quad & 5\int \cos(-x)\,dx + \int \sin(3x)\,dx \\ & = 5 \times \frac{\sin(-x)}{-1} + \frac{-\cos(3x)}{3} + C \\ & = -5\sin(-x) - \frac{\cos(3x)}{3} + C\end{aligned}$$

5.5 Finding the Constant of Integration

In the integrals so far we have always had a constant of integration denoted $+C$ at the end. Consider the functions $y = x^2$, $y = x^2 + 2$ and $y = x^2 - 5$, as shown on the graph below. These all differentiate to $2x$. So when integrating $2x$ we don't know whether the actual answer is $y = x^2$, $y = x^2 + 2$ or $y = x^2 - 5$ so we give the general answer of $y = x^2 + C$.



If we are given the gradient of a curve and a point that the curve goes through, we can find full equation of the curve and therfore a value of C.

Example: A curve of gradient $4x^5$ passes through the point (1, 2). What is the full equation of the line?

Solution: We know the gradient is $4x^5$ meaning $\dfrac{dy}{dx} = 4x^5$. Hence we have:

$$\begin{aligned} y &= \int 4x^5\,dx && \text{Now can integrate} \\ y &= \frac{4}{6}x^6 + C && \text{Simplify the fraction} \\ y &= \frac{2}{3}x^6 + C \end{aligned}$$

We now have an expression for y in terms of x however it has a constant C in it. Since we know a point $(1, 2)$ that the curve passes through we can find this constant. So when $x = 1$ we have $y = 2$ substituting this into the equation gives:

$$\begin{aligned} 2 &= \frac{2}{3} \times 1^6 + C && \text{Rearrange to find } C \\ \frac{4}{3} &= C \end{aligned}$$

We now substitute the value of C into the equation from before to find our answer:

$$y = \frac{2}{3}x^6 + \frac{4}{3}$$

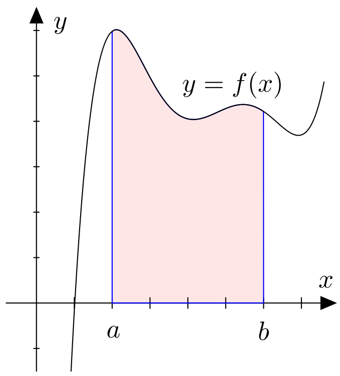
5.6 Integrals with Limits

Integrals represent the area under a graph. The probability of finding an electron between two points or the energy needed to separate two atoms can be represented as the area under the curve and we can use integration to find their value. **Definite integrals** are ones evaluated between two values (or limits):

$$\boxed{\int_a^b f(x)\,dx = \Big[F(x)\Big]_a^b = F(b) - F(a)}$$

- The braces $\Big[..\Big]_a^b$ with a and b signify that we will evaluate the integral between these two limits.
- The numerical answer produced by $F(b) - F(a)$ represents the area under the curve.

Below is a function $f(x)$ integrated between the limits a and b with the shaded area being $\displaystyle\int_a^b f(x)\,dx$



Note: There is no need to find C when doing this since they cancel out. When evaluating between the two points we will have $\big(F(b)+C\big) - \big(F(a)+C\big) = F(b) - F(a) + C - C = F(b) - F(a)$

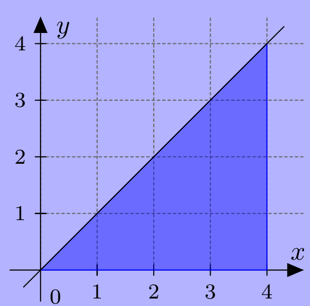
Example: Calculate $\displaystyle\int_0^4 x\,dx$

Solution: We first integrate with respect to x.

$$\int_0^4 x\,dx = \left[\frac{1}{2}x^2\right]_0^4 \qquad \text{Substitute the limits in}$$

$$\left[\frac{1}{2}x^2\right]_0^4 = \left[\frac{1}{2}\times 4^2\right] - \left[\frac{1}{2}\times 0\right] \qquad = 8$$

We can verify this answer by seeing that the area in question is a triangle below.



We could have easily found the area of the triangle without integration but when we have more complicated functions then we must use integration.

Example: Find $\displaystyle\int_0^{\pi} \sin(x)\,dx$

Click here for a video example

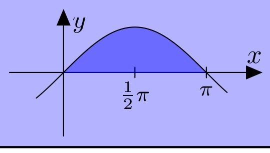
Solution: To begin we will integrate the function:

$$\int_0^{\pi} \sin(x)\,dx = \Big[-\cos(x)\Big]_0^{\pi} \qquad \text{Evaluate this at the limits}$$

$$\Big[-\cos(x)\Big]_0^{\pi} = \big(-\cos(\pi)\big) - \big(-\cos(0)\big) \qquad \text{Put those cosines into numbers}$$

$$\big(-\cos(\pi)\big) - \big(-\cos(0)\big) = -(-1) + 1 = 2$$

The integral is 2, which means that the area under the curve from 0 to π is 2 as shown below.



Chemistry Example: 2.0 moles of an ideal gas is compressed isothermally to half of it's initial volume. This process happens at 300K. The work done on the gas is given by the equation:

$$W_{\text{on}} = -\int_{V_1}^{V_2} P\,dV$$

where V_1 and V_2 are the initial and final volumes respectively. By using the ideal gas equation and integration, find the amount of work done on the gas.

Click here for a video example

Solution: We start by relating the initial and final volumes. Since the end volume is half that of the start we can write $V_1 = 2V_2$. This will be important later on.

Now we tackle this integral in which P is being integrated with respect to V hence we need to find an expression for P in terms of V. From the ideal gas equation we know $PV = nRT$ so we make P the subject of the formula. Dividing through by V gives:

$$P = \frac{nRT}{V}$$

Substituting this and our limits into the integral gives:

$$W_{\text{on}} = -\int_{2V_2}^{V_2} \frac{nRT}{V}\,dV \qquad \text{The constants can be taken outside of the integral}$$

$$W_{\text{on}} = -nRT\int_{2V_2}^{V_2} \frac{1}{V}\,dV \qquad \text{Integrate } \frac{1}{V} \text{ in the limits}$$

$$W_{\text{on}} = -nRT\Big[\ln(V)\Big]_{2V_2}^{V_2} \qquad \text{Evaluate the integral between the limits}$$

$$W_{\text{on}} = -nRT\Big[\ln(V_2) - \ln(2V_2)\Big] \qquad \text{Using the laws of logs this simplifies to a single log}$$

$$W_{\text{on}} = -nRT\ln\left(\frac{V_2}{2V_2}\right) \qquad \text{Simplify further}$$

$$W_{\text{on}} = -nRT\ln(\tfrac{1}{2}) \qquad \text{Put the numbers in to get a final answer}$$

$$W_{\text{on}} = -2.0 \times 300 \times 8.31 \times \ln(\tfrac{1}{2}) \qquad = 3.456\ldots \times 10^3 \text{ J} = 3.5 \times 10^3 \text{ J (to 2 s.f.)}.$$

5.7 Separating the Variables

A differential equation is an equation of the form:

$$\boxed{\frac{dy}{dx} = f(x, y)}$$

where $f(x, y)$ is a function of x and y. The method of separating the variables works by getting our differential equation into the form:

$$\boxed{f_1(y)\, dy = f_2(x)\, dx}$$

so we have all the ys on the left hand side of the equation and the xs on the right hand side then we can integrate as below.

$$\boxed{\int f_1(y)\, dy = \int f_2(x)\, dx}$$

Example: If $\dfrac{dy}{dx} = 4x^3$ then use the method of separation of variables to integrate with respect to x.

Solution: So first we need to get the differential equation into the correct form with all the x's on the right hand side and all the y's on the left. Multiplying both sides by y^2 gives:

$$dy = 4x^3\, dx$$

We can now integrate both sides, the left with respect to y and the right with respect to x:

$$\begin{aligned} \int dy &= \int 4x^3\, dx && \text{Complete the integrals} \\ y &= \frac{4x^4}{4} + C && \text{Simplify} \\ y &= x^4 + C \end{aligned}$$

Example: If $\dfrac{dy}{dx} = \dfrac{\sin(-x) + e^{4x}}{y^2}$ then use the method of separation of variables to find an expression for y in terms of x.

Solution: So first we need to get the differential equation into the correct form will all the x's on the right hand side and all the y's on the left. So we have:

$$y^2\, dy = \big(\sin(-x) + e^{4x}\big)\, dx$$

We can now integrate both sides, the left with respect to y and the right with respect to x:

$$\begin{aligned} \int y^2\, dy &= \int \left(\sin(-x) + e^{4x}\right) dx && \text{Split up the integral on the right} \\ \int y^2\, dy &= \int \sin(-x)\, dx + \int e^{4x}\, dx && \text{Integrate both sides} \\ \frac{y^3}{3} &= \cos(-x) + \frac{e^{4x}}{4} + C && \text{Multiply both sides by 3} \\ y^3 &= \frac{3}{4}e^{4x} + 3\cos(-x) + 3C && \text{Take the cube root of both sides} \\ y &= \left(\frac{3}{4}e^{4x} + 3\cos(-x) + C'\right)^{\frac{1}{3}} && \text{Where } C' = 3C \end{aligned}$$

Chemistry Example: In a reaction mixture at a fixed temperature the concentration of a reactant [A] varies with time t according to the differential equation:

$$\frac{d[\mathrm{A}]}{dt} = -2k[\mathrm{A}]^2$$

Integrate the equation with the boundary limits that when $t = 0$ and $[\mathrm{A}] = [\mathrm{A}]_0$ to get the following equation.

$$\frac{1}{[\mathrm{A}]} - \frac{1}{[\mathrm{A}]_0} = 2kt$$

Solution: First we need to put all the [A]'s on the left and t's on the right to give:

$$\frac{1}{[\mathrm{A}]^2}\, d[\mathrm{A}] = -2k\, dt$$

We can now apply the integral both sides:

$$\int \frac{1}{[\mathrm{A}]^2}\, d[\mathrm{A}] = \int -2k\, dt \qquad \text{Change } \frac{1}{[\mathrm{A}]^2} \text{ to } [\mathrm{A}]^{-2}$$

$$\int [\mathrm{A}]^{-2}\, d[\mathrm{A}] = \int -2k\, dt \qquad \text{Integrate both sides}$$

$$-[\mathrm{A}]^{-1} = -2kt + C$$

Now we can substitute in our limits to find C. When $t = 0$ and $[\mathrm{A}] = [\mathrm{A}]_0$ we have:

$$-[\mathrm{A}]_0{}^{-1} = -2k \times 0 + C \qquad \text{Simplify}$$

$$C = -[\mathrm{A}]_0{}^{-1}$$

Substituting this C back into our equation obtained by the integral gives:

$$-[\mathrm{A}]^{-1} = -2kt - [\mathrm{A}]_0{}^{-1} \qquad \text{Rearrange to get it into the form required}$$

$$\frac{1}{[\mathrm{A}]} - \frac{1}{[\mathrm{A}]_0} = 2kt$$

Chemistry Example: In electrochemistry the Cottrell equation:

$$I = nFAc\sqrt{\frac{D}{\pi}}\,t^{-\frac{1}{2}}$$

describes the current I at a time t after an electrode is immersed in solution. Current is defined as the rate of change of charge Q so:

$$I = \frac{dQ}{dt}.$$

Using this find an expression for charge.

Solution: Since $I = \dfrac{dQ}{dt}$ we can substitute this into the equation involving t to form a differential equation:

$$\frac{dQ}{dt} = nFAc\sqrt{\frac{D}{\pi}}\,t^{-\frac{1}{2}} \qquad \text{Multiply both sides by } dt$$

$$dQ = nFAc\sqrt{\frac{D}{\pi}}\,t^{-\frac{1}{2}}\,dt \qquad \text{Integrate both sides of the equation}$$

$$\int dQ = \int nFAc\sqrt{\frac{D}{\pi}}\,t^{-\frac{1}{2}}\,dt \qquad \text{Since } n, F, A, c \text{ and } D \text{ are constants they can be taken out of the integral}$$

$$\int dQ = nFAc\sqrt{\frac{D}{\pi}}\int t^{-\frac{1}{2}}\,dt \qquad \text{Integrate both sides}$$

$$Q = nFAc\sqrt{\frac{D}{\pi}} \times \frac{t^{-\frac{1}{2}+1}}{-\frac{1}{2}+1} + C \qquad \text{Then simplify}$$

$$Q = nFAc\sqrt{\frac{D}{\pi}}\,2t^{\frac{1}{2}} + C$$

Chemistry Example: The force between two particles is modelled to be:

$$F = \frac{12\varepsilon}{a_0}\left[\left(\frac{a_0}{r}\right)^{13} - \left(\frac{a_0}{r}\right)^{7}\right]$$

Given that force is the negative derivative of potential, i.e. $F = -\dfrac{d}{dr}U$, and at $r = a_0$, $U = -\varepsilon$ calculate the potential between the two particles.

Solution: This is a problem of seperating variables so first we set up the problem:

$$-\frac{d}{dr}U = \frac{12\varepsilon}{a_0}\left[\left(\frac{a_0}{r}\right)^{13} - \left(\frac{a_0}{r}\right)^{7}\right] \qquad \text{Turn this into a nicer form with negative powers}$$

$$-\frac{d}{dr}U = \frac{12\varepsilon}{a_0}\left[a_0^{13}\,r^{-13} - a_0^{7}\,r^{-7}\right] \qquad \text{Multiply by } dr \text{ and integrate both sides}$$

$$-\int dU = \int \frac{12\varepsilon}{a_0}\left[a_0^{13}\,r^{-13} - a_0^{7}\,r^{-7}\right] dr \qquad \text{Take the constant } \frac{12\varepsilon}{a_0} \text{ out of the integral}$$

$$-U = \frac{12\varepsilon}{a_0}\int \left[a_0^{13}\,r^{-13} - a_0^{7}\,r^{-7}\right] dr \qquad \text{Now integrate the right hand side}$$

$$-U = \frac{12\varepsilon}{a_0}\left(-\frac{a_0^{13}}{12}r^{-12} + \frac{a_0^{7}}{6}r^{-6}\right) + C \qquad \text{This simplifies down}$$

$$U = \varepsilon\big(a_0^{12}\,r^{-12} - 2a_0^{6}\,r^{-6}\big) + C$$

Now find C by substitution $(r = a_0, U = -\varepsilon)$

$$-\varepsilon = \varepsilon\big(a_0^{12}\,a_0^{-12} - 2a_0^{6}\,a_0^{-6}\big) + C \qquad \text{Simplify this}$$

$$-\varepsilon = \varepsilon\big(1 - 2\big) + C$$

$$-\varepsilon = -\varepsilon + C$$

$$0 = C$$

Back into our equation we get, $U = \varepsilon\big(a_0^{12}\,r^{-12} - 2a_0^{6}\,r^{-6}\big)$.

Note: This is another form of the Lennard-Jones 6-12 potential, with a_0 being the equilibrium seperation and ε being the energy needed to move the particles apart to infinity.

6 Vectors

6.1 Introduction to Vectors

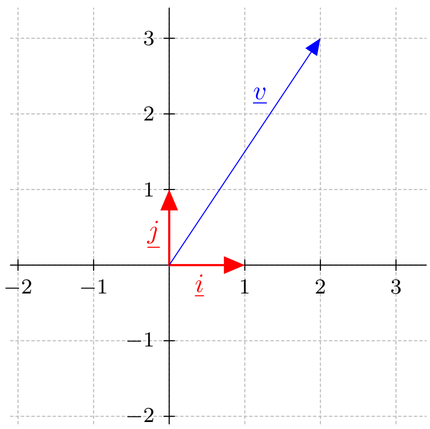
When describing some quantities just a number and units aren't enough. Say we are navigating a ship across the ocean and we are told that the port is 5km away we don't know in which direction we have to sail. 5km due east would give us all the information that we need. This is an example of a **vector**, a quantity that has *magnitude* and *direction*.

- Some chemistry related vector quantities are velocity, force, acceleration, linear and angular momentum and electric and magnetic fields.
- Quantities that have just a *magnitude* are **scalars**. Examples of these are temperature, mass and speed.

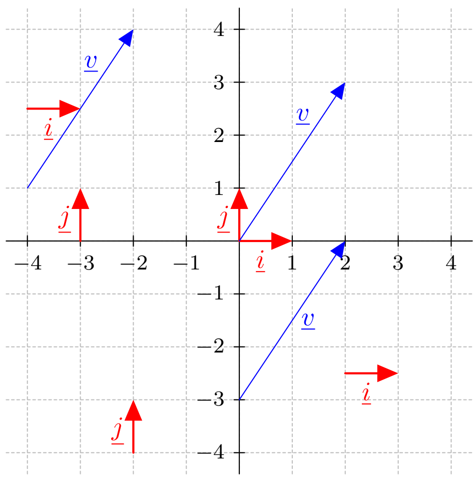
Note: To distinguish vectors from scalars we write them with a line under them, e.g. $\underline{F}$ is used as the symbol for a force vector. Some books will use bold font for this e.g. **F**.

Vectors in 2-D Space

A vector in 2-D space can be written as a combination of 2 base vectors, $\underline{i}$ being a horizontal vector (in the x direction) and $\underline{j}$ being a vertical vector (in the y direction). They are both unit vectors meaning that their length (magnitude) is 1. For an example the vector $\underline{v} = 2\underline{i} + 3\underline{j}$ is shown below:



Note: The vector $\underline{v}$ above also describes all vectors that move 2 $\underline{i}$ units and 3 $\underline{j}$ units, they don't have to start at the origin. All the vectors in the graph below are exactly the same:

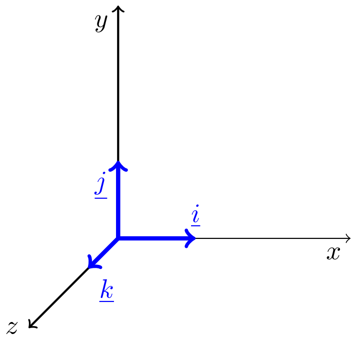


Writing a general 2-D vector $\underline{u}$ as a combination of the unit vectors would give:

$$\underline{u} = a\underline{i} + b\underline{j}$$
Where a and b are real numbers

Vectors in 3-D Space

Any vector in 3-D space can be written as a combination of 3 base vectors; $\underline{i}$, $\underline{j}$ and $\underline{k}$ each being the unit vector in the x, y and z directions. Below is a graph of the 3 axes with their respective unit vectors:



Writing a general vector $\underline{v}$ as a combination of the unit vectors would give:

$$\underline{v} = a\underline{i} + b\underline{j} + c\underline{k}$$
Where a, b and c are real numbers

Representation of Vectors

A vector $\underline{v}$ can be written in the following forms:

1. **Unit vector notation:**

$$\boxed{\underline{v} = a\underline{i} + b\underline{j} + c\underline{k}}$$

   The vector is displayed as the clear sum of it's base vectors. In 3-D space those are the $\underline{i}$, $\underline{j}$ and $\underline{k}$ vectors.

2. **Ordered set notation:**

$$\boxed{\underline{v} = (a, b, c)}$$

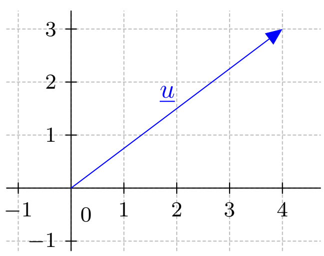
   The vector is in the same form as unit vector notation (a, b and c are the same numbers) but it is more compact.

3. **Column notation:**

$$\boxed{\underline{v} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}}$$

   This is identical to ordered set notation apart from it being vertical. This form makes some calculations easier to visualise, such as the dot product.

For example, the 2-D vector $\underline{u}$ shown below can be written as $\underline{u} = 4\underline{i} + 3\underline{j}$ or $\underline{u} = (4, 3)$ or $\underline{u} = \begin{pmatrix} 4 \\ 3 \end{pmatrix}$



Magnitude of Vectors

If we know the lengths of each of the component vectors we can find the length (or magnitude) of the vector using Pythagoras:

$$\text{For a vector } \underline{v} = a\underline{i} + b\underline{j} + c\underline{k}$$
$$\text{Magnitude of } \underline{v} = |\,\underline{v}\,| = \sqrt{a^2+b^2+c^2}$$

For vector $\underline{u} = 4\underline{i}+3\underline{j}$ above we can calculate the magnitude $|\,\underline{u}\,|$ to be $\sqrt{4^2+3^2} = \sqrt{16+9} = \sqrt{25} = 5$

Example: Find the magnitude of the following vectors:

1. $(2, 6, 3)$
2. $\underline{i} + 7\underline{j} + 4\underline{k}$
3. $\begin{pmatrix} \sqrt{2} \\ \sqrt{2} \\ 0 \end{pmatrix}$

Solution:

1. $|\,(2,6,3)\,| = \sqrt{2^2+6^2+3^2} = \sqrt{4+36+9} = \sqrt{49} = 7$
2. $|\underline{i} + 7\underline{j} + 4\underline{k}\,| = \sqrt{1^2+7^2+4^2} = \sqrt{1+49+16} = \sqrt{66}$
3. $\left|\begin{pmatrix} \sqrt{2} \\ \sqrt{2} \\ 0 \end{pmatrix}\right| = \sqrt{\sqrt{2}^2+\sqrt{2}^2} = \sqrt{2+2} = \sqrt{4} = 2$

Chemistry Example: A helium atom is moving with a velocity $\underline{v}$ of $20\underline{i} - 15\underline{j}$ m/s. What is it's speed?

Solution: Since speed is the magnitude of velocity, we take the magnitude of the velocity vector. This gives:

$$|\,20\underline{i} - 15\underline{j}\,| = \sqrt{20^2+15^2} = \sqrt{625} = 25$$

The particle's speed is 25 m/s

6.2 Operations with Vectors

Scalar Multiplication

Scalar multiplication is when we multiply a vector by a scalar. We do this by multipling each component of the vector by the scalar. This can be expressed as:

$$\lambda \times (x, y, z) = (\lambda x, \lambda y, \lambda z)$$

Where λ is a real number

Note: Scalar multiplication only changes the magnitude of the vector while the direction stays the same.

Example: Simplify $7(-12, 4)$

Solution: We multiply each component of the vector by 7 giving:

$$(7 \times -12,\ 7 \times 4) = (-84, 28)$$

Vector Addition and Subtraction

When we add or subtract two vectors we add or subtract each of the individual compoments of the vectors. This can be expressed as:

$$(a, b, c) + (x, y, z) = (a + x,\ b + y,\ c + z)$$

Where (a, b, c) and (x, y, z) are both vectors using $\underline{i}$, $\underline{j}$ and $\underline{k}$.

IMPORTANT: If the vectors have a different number of base components, for example $(3, 6) + (1, 0, 7)$ we can not complete the addition. For all vector on vector operations both vectors need to have the same number of base components.

Example: Calculate the following:

1. $(2, 2, 0) + (5, -1, 3)$
2. $3(a, 4a, 0) - a(7, 0, -1)$
3. $(1, 3, 8) + (2, 1, -5) + (-1, 2, -1)$

Solution:

1. $(2, 2, 0) + (5, -1, 3) = (2 + 5,\ 2 - 1,\ 0 + 3) = (7, 1, 3)$
2. $3(a, 4a, 0) - a(7, 0, -1) = (3a, 12a, 0) - (7a, 0, -a) = (3a - 7a,\ 12a - 0,\ 0 + a) = (-4a, 12a, a)$
3. $(1, 3, 8) + (2, 1, -5) + (-1, 2, -1) = (1 + 2 - 1,\ 3 + 1 + 2,\ 8 - 5 - 1) = (2, 6, 2)$

Vector Multiplication: Dot Product

There are two ways of multiplying two vectors together. The first is the dot (or scalar) product which is defined to be:

$$\underline{A} \cdot \underline{B} = |\,\underline{A}\,|\,|\,\underline{B}\,|\cos\theta$$

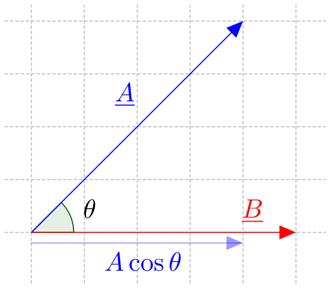
Where θ is the angle between vectors $\underline{A}$ and $\underline{B}$

IMPORTANT: Taking the dot product of two vectors produces a scalar quantity.

Given two vectors, the dot product can also be calculated in the following way:

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} \bullet \begin{pmatrix} x \\ y \\ z \end{pmatrix} = ax + by + cz$$

Note: The dot product can be thought of how much one vector is pointing in the direction of the other.



The part of $\underline{A}$ that goes in the same direction as $\underline{B}$ has a length of $|\underline{A}|\cos\theta$, making the dot product the length of $\underline{B}$ times the length of $\underline{A}$ that is in the same direction as $\underline{B}$

Example: Calculate the following:

1. $\begin{pmatrix} 3 \\ 9 \\ 1 \end{pmatrix} \bullet \begin{pmatrix} 1 \\ -2 \\ 10 \end{pmatrix}$

2. $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \bullet \begin{pmatrix} \sqrt{2} \\ \sqrt{2} \end{pmatrix}$

Solution:

1. $\begin{pmatrix} 3 \\ 9 \\ 1 \end{pmatrix} \bullet \begin{pmatrix} 1 \\ -2 \\ 10 \end{pmatrix} = 3 \times 1 + 9 \times (-2) + 1 \times 10 = 3 - 18 + 10 = -5$

2. $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \bullet \begin{pmatrix} \sqrt{2} \\ \sqrt{2} \end{pmatrix} = 1 \times \sqrt{2} + 0 \times \sqrt{2} = \sqrt{2}$

Chemistry Example: An ion moving through solution has 2 forces acting upon it, a resistive force from the medium with a vector of $(3, \sqrt{7}, 3)$ and an electromagnetic force from an electric field with a vector of $(-5, 3, 4)$. What is the angle between these two vectors?

Solution: To calculate this we find the dot product of the two vectors and then employ the definition of the dot product to find the angle. The dot product of the two vectors is:

$$\begin{pmatrix} 3 \\ \sqrt{7} \\ 3 \end{pmatrix} \bullet \begin{pmatrix} -5 \\ 3 \\ 4 \end{pmatrix} = 3 \times (-5) + \sqrt{7} \times 3 + 3 \times 4 \qquad \text{Simplify this}$$

$$= -15 + 3\sqrt{7} + 12 = -3 + 3\sqrt{7} = 3(\sqrt{7} - 1) \approx 4.937$$

Using the definition $\underline{A} \cdot \underline{B} = |\,\underline{A}\,||\,\underline{B}\,| \cos\theta$ we can now find out what θ is. First we must find the magnitudes of the two vectors:

$$|(3, \sqrt{7}, 3)| = \sqrt{3^2 + 7 + 3^2} = \sqrt{25} = 5 \qquad \text{For the first vector}$$

$$|(-5, 3, 4)| = \sqrt{(-5)^2 + 3^2 + 4^2} = \sqrt{50} = 5\sqrt{2} \qquad \text{For the second vector}$$

Putting all this information into the equation $\underline{A} \cdot \underline{B} = |\,\underline{A}\,||\,\underline{B}\,| \cos\theta$ gives us:

$$3(\sqrt{7} - 1) = 5 \times 5\sqrt{2} \cos\theta \qquad \text{Rearrange for } \cos\theta$$

$$\frac{3(\sqrt{7} - 1)}{25\sqrt{2}} = \cos\theta \qquad \text{Take the arccos of both sides}$$

$$\theta = \arccos(0.1396\ldots) = 81.97^\circ \cdots = 82.0^\circ \text{ to 3 s.f.}$$

Chemistry Example: What is the work done w by the vector force $\underline{F} = (3t\underline{i} + 3\underline{j})\,\text{N}$ on a particule of velocity $\underline{v} = (5\underline{i} - t\underline{j})\,\text{ms}^{-1}$ in the time interval $0 < t < 3\,\text{s}$ given that:

$$w = \int_0^3 F \cdot v \, dt$$

Solution: First we must find the dot product $F \cdot v$.

$$F \cdot v = (3t\underline{i} + 3\underline{j}) \cdot (5\underline{i} - t\underline{j}) = 3t \times 5 + 3 \times (-t) = 12t$$

Now we have found the dot product we can substitute it in the integral and solve.

$$\begin{aligned} w &= \int_0^3 F \cdot v \, dt \\ &= \int_0^3 12t \, dt \\ &= \Big[6t^2\Big]_0^3 \\ &= \Big[6 \times 3^2\Big] - \Big[6 \times 0^2\Big] = 54\,\text{J} \end{aligned}$$

Vector Multiplication: Cross Product

The cross product (or vector product) is defined to be:

$$\underline{A} \times \underline{B} = |\,\underline{A}\,|\,|\,\underline{B}\,| \sin\theta\ \hat{\underline{n}}$$

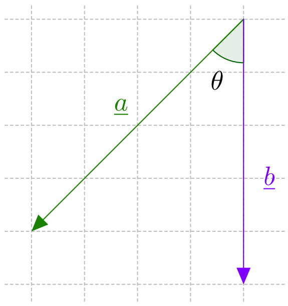
Where θ is the angle between the two vectors and $\hat{\underline{n}}$ is the unit vector in the direction of the new vector.

IMPORTANT: The cross product takes two vectors and produces a new vector. This new vector is in the direction **perpendicular** to the plane that $\underline{A}$ and $\underline{B}$ are in. It is only possible to take the cross product of two 3-D vectors (and technically 7-D vectors as well).

The cross product is also dependent on the order of the vectors appear in the product. If we change the order of the vectors in a cross product then our answer becomes negative. The vector points in the opposite direction.

$$\boxed{\underline{a} \times \underline{b} = -\underline{b} \times \underline{a}}$$

The right hand rule determines which way the vector produced will point. We use the rule as follows: curl your fingers from the first vector in the cross product to the second vector and the direction your thumb points is the direction of the vector produced by the cross product.



In this case, $\underline{a} \times \underline{b}$ will point out of the page and $\underline{b} \times \underline{a}$ will point into the page.

Calculating the Cross Product

When using the standard base vectors of $\hat{\underline{i}}$, $\hat{\underline{j}}$ and $\hat{\underline{k}}$, we can calculate the cross product by considering the cross product of the base vectors with each other:

$$\boxed{\underline{i} \times \underline{i} = \underline{j} \times \underline{j} = \underline{k} \times \underline{k} = \underline{0}}$$

$$\boxed{\underline{i} \times \underline{j} = -\underline{j} \times \underline{i} = \underline{k}}$$

$$\boxed{\underline{j} \times \underline{k} = -\underline{k} \times \underline{j} = \underline{i}}$$

$$\boxed{\underline{k} \times \underline{i} = -\underline{i} \times \underline{k} = \underline{j}}$$

Taking the cross products of two vectors is just like expanding brackets. The cross product two general vectors, $(a\underline{i} + b\underline{j} + c\underline{k}) \times (x\underline{i} + y\underline{j} + z\underline{k})$, would give $ax(\underline{i} \times \underline{i}) + ay(\underline{i} \times \underline{j}) + az(\underline{i} \times \underline{k}) + \ldots$ Fully expanded and simplified gives:

$$(a\underline{i} + b\underline{j} + c\underline{k}) \times (x\underline{i} + y\underline{j} + z\underline{k}) = (bz - cy)\underline{i} + (cx - az)\underline{j} + (ay - bx)\underline{k}$$

Where a, b, c, x, y and z are real numbers

Example: Calculate the following cross product:

$$\begin{pmatrix} 3 \\ 1 \\ -2 \end{pmatrix} \times \begin{pmatrix} 2 \\ -1 \\ 1 \end{pmatrix}$$

Solution: So to find this we use the formula below:

$$\left(a\underline{i} + b\underline{j} + c\underline{k}\right) \times \left(x\underline{i} + y\underline{j} + z\underline{k}\right) = \left(bz - cy\right)\underline{i} + \left(cx - az\right)\underline{j} + \left(ay - bx\right)\underline{k}$$

Now we can write the vectors in the question in the form of the rule so $\left(a\underline{i}+b\underline{j}+c\underline{k}\right) = \left(3\underline{i}+1\underline{j}-2\underline{k}\right)$ and $\left(x\underline{i} + y\underline{j} + z\underline{k}\right) = \left(2\underline{i} - 1\underline{j} + 1\underline{k}\right)$

Hence $a = 3$, $b = 1$, $c = -2$, $x = 2$, $y = -1$ and $z = 1$ and therefore:

$$\begin{aligned} &\left(3\underline{i} + 1\underline{j} - 2\underline{k}\right) \times \left(2\underline{i} - 1\underline{j} + 1\underline{k}\right) \\ &= \left(1 \times 1 - (-2) \times (-1)\right)\underline{i} + \left((-2) \times 2 - 3 \times 1\right)\underline{j} + \left(3 \times (-1) - 1 \times 2\right)\underline{k} \\ &= -1\underline{i} - 7\underline{j} - 5\underline{k} \end{aligned}$$

This could also be written:

$$\begin{pmatrix} 3 \\ 1 \\ -2 \end{pmatrix} \times \begin{pmatrix} 2 \\ -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ -7 \\ -5 \end{pmatrix}$$

7 Complex Numbers

7.1 Imaginary Numbers

Imaginary numbers allow us to find an answer to the question 'what is the square root of a negative number?' We define i to be the square root of minus one.

$$\boxed{i = \sqrt{-1}}$$

We find the other square roots of a negative number say $-x$ as follows:

$$\boxed{\sqrt{-x} = \sqrt{x \times -1} = \sqrt{x} \times \sqrt{-1} = \sqrt{x} \times i}$$

Example: Find the square root of:

1. $\sqrt{-9}$
2. $\sqrt{-13}$

Solution:

1. $\sqrt{-9} = \sqrt{9 \times -1} = \sqrt{9} \times \sqrt{-1} = 3i$
2. $\sqrt{-13} = \sqrt{13 \times -1} = \sqrt{13} \times \sqrt{-1} = \sqrt{13}\, i$

7.2 Complex Numbers

A complex number is a number that has both a real and imaginary component. They can be written in the form:

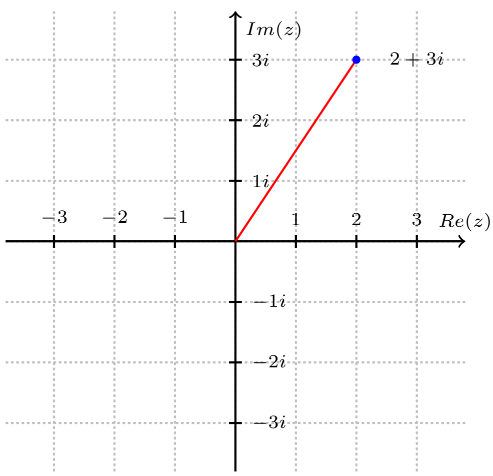
$$\boxed{a + bi}$$

where a and b are real numbers and $i = \sqrt{-1}$.

We often denote complex numbers by the letter z so $z = a + bi$.

- a is the real part of z we denote this $Re(z) = a$.
- b is the imaginary part of z we denote this $Im(z) = a$.
- $z^* = a - bi$ is called the complex conjugate of $z = a + bi$

Just as we have a number line for real numbers we can draw complex numbers on an x, y axis called an Argand diagram with imaginary numbers on the y-axis and real numbers on the x-axis. We have drawn $2 + 3i$ on the Argand diagram below.



Example: Find the imaginary and real parts of the following complex numbers along with their complex conjugates.

1. $z = -3 + 5i$
2. $z = 1 - 2\sqrt{3}\,i$
3. $z = i$

Solution:

1. For $z = -3 + 5i$ we have $Re(z) = -3$, $Im(z) = 5$ and $z^* = -3 - 5i$
2. For $z = 1 + 2\sqrt{3}\,i$ we have $Re(z) = 1$, $Im(z) = -2\sqrt{3}$ and $z^* = 1 + 2\sqrt{3}\,i$
3. For $z = i$ we have $Re(z) = 0$, $Im(z) = 1$ and $z^* = -i$

Different Forms for Complex Numbers

When a complex number z is in the form $z = a + bi$ we say it is written in Cartesian form. We can also write complex numbers in:

- Polar form: $r(\cos(\phi) + i\sin(\phi))$
- Exponential form: $re^{i\phi}$

where the magnitude $|z|$ (or modulus) of z is the length r.

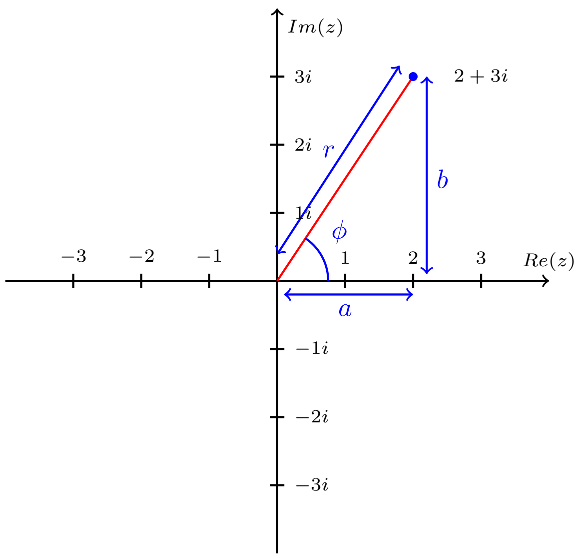
$$\boxed{|z| = r = \sqrt{a^2 + b^2}}$$

and the argument of z is the angle ϕ (this must be in radians).

$$\boxed{\arg(z) = \phi = \tan^{-1}\left(\frac{b}{a}\right)}$$

This argument ϕ is usually between $-\pi$ and π. Expressed mathematically this is $-\pi < \phi \leq \pi$.

We can see on an Argand diagram the relationship between the different forms for representing a complex number.



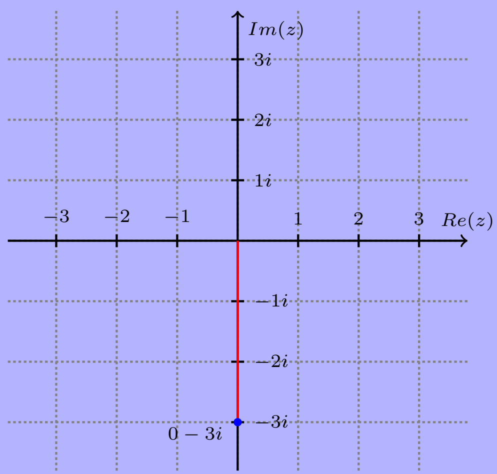
Example: Find the modulus and argument of the following complex numbers:

1. $3+3i$
2. $-4+3i$
3. $-3i$
4. 4

Solution:

1. For $3+3i$ we have $|z| = \sqrt{3^2+3^2} = \sqrt{18}$ and $arg(z) = \tan^{-1}\left(\frac{3}{3}\right) = \frac{\pi}{4}$ radians.
2. For $-4+3i$ we have $|z| = \sqrt{(-4)^2+(3)^2} = 5$ and $arg(z) = \tan^{-1}\left(\frac{3}{-4}\right) = -0.64$ radians.
3. For $-3i$ we have $|z| = \sqrt{0^2+(-3)^2} = 3$ and $arg(z) = \tan^{-1}\left(\frac{-3}{0}\right)$

   This calculation does not make sense since we can't divide by zero. However from plotting $-3i$ on an Argand diagram the argument is clearly $arg(z) = \frac{-\pi}{2}$ radians.



4. For 4 we have $|z| = \sqrt{4^2+0^2} = 4$ and $arg(z) = \tan^{-1}\left(\frac{0}{4}\right) = 0$ radians.

Example: Express $4-5i$ in polar and exponential form.

Solution: First we need to find the modulus and argument.

$|z| = r = \sqrt{4^2+(-5)^2} = \sqrt{41}$ and $arg(z) = \phi = \tan^{-1}\left(\frac{-5}{4}\right) = -0.90$ radians

So in polar form $r(\cos(\phi)+i\sin(\phi))$ we have $\sqrt{41}(\cos(-0.90)+i\sin(-0.90))$.

In exponential form $re^{i\phi}$ we have $\sqrt{41}e^{-0.90\,i}$.

Chemistry Example: Written in Exponential form the radial wave function for a 2p orbital of hydrogen is:

$$\psi_{2p} = \mp\frac{1}{\sqrt{2}} r\sin(\theta)e^{\pm i\phi} f(r)$$

Write this in Polar form.

Solution: A complex number in Exponential form: $re^{i\phi}$ has Polar form: $r(\cos(\phi) + i\sin(\phi))$.

Because of the $\mp$ and $\pm$ signs in this question we have either:

$$r = \frac{1}{\sqrt{2}} r\sin(\theta)f(r) \text{ and } \phi = -\phi$$

OR

$$r = -\frac{1}{\sqrt{2}} r\sin(\theta)f(r) \text{ and } \phi = \phi$$

Hence in Polar form we have either:

$$r = \frac{1}{\sqrt{2}} r\sin(\theta)f(r)(\cos(-\phi) + i\sin(-\phi))$$

OR

$$r = -\frac{1}{\sqrt{2}} r\sin(\theta)f(r)(\cos(\phi) + i\sin(\phi))$$

Applications

When using the quadratic formula:

$$\frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

we would not have known what to do if $b^2 - 4ac$ was negative however now we are able to solve this square root using imaginary numbers.

Example: Solve the equation $x^2 + 3x + 12$ using the quadratic formula

Solution: So we have that $a = 1$, $b = 3$ and $c = 12$ so the quadratic formula gives:

$$\begin{aligned}\frac{-b \pm \sqrt{b^2 - 4ac}}{2a} &= \frac{-3 \pm \sqrt{3^2 - 4 \times 1 \times 12}}{2 \times 1}\\ &= \frac{-3 \pm \sqrt{-39}}{2}\\ &= \frac{-3 \pm i\sqrt{39}}{2}\end{aligned}$$

This gives us $x = \dfrac{-3 + i\sqrt{39}}{2}$ and $x = \dfrac{-3 - i\sqrt{39}}{2}$.

Note: The two roots are complex conjugates of each other.

7.3 Arithmetic of Complex Numbers

If we have two complex numbers $a+bi$ and $c+di$ then we have the following rules for the arithmetic of complex numbers:

1. **Addition:** $(a+bi)+(c+di)=(a+c)+(b+d)i$
   Add the real parts and add the complex parts separately.

2. **Subtraction:** $(a+bi)-(c+di)=(a-c)+(b-d)i$
   Same as addition but with subtraction.

3. **Multiplication:** $(a+bi)(c+di)=(ac-bd)+(ad+bc)i$
   Treat it as 2 set of brackets and use FOIL. Remember that $i^2=-1$.

4. **Division:** $\dfrac{a+bi}{c+di}=\dfrac{ac+bd}{c^2+d^2}+\dfrac{bc-ad}{c^2+d^2}i$
   Multiply the numerator and denominator by the conjugate of the denominator. This makes the denominator a real number and the numerator the multiplication of two complex numbers.

Example: Find the following:

1. $(2+i)+(1-i)$
2. $(-4-4i)-(-5i)$
3. $(1+i)(2-3i)$
4. $\dfrac{1-i}{2+3i}$

Solution:

1. $(2+i)+(1-i)=(2+1)+(1-1)i=3$
2. $(-4-4i)-(-5i)=(-4-0)+(-4-(-5))i=-4+i$
3. $(1+i)(2-3i)=((1\times 2)-(1\times -3))+((1\times -3)+(1\times 2))i=5-i$
4. $\dfrac{1-i}{2+3i}=\dfrac{(1\times 2)+(-1\times 3)}{2^2+3^2}+\dfrac{(-1\times 2)-(1\times 3)}{2^2+3^2}i=\dfrac{-1}{13}-\dfrac{5}{13}i$

Chemistry Example: A particle is described by a wavefunction Ψ. To calculate the probability of finding this particle somewhere $\Psi\Psi^*$ needs to be caclulated. When Ψ is in the form:

$$\Psi = a+bi$$

calculate $\Psi\Psi^*$.

Solution: Since $\Psi=a+bi$, this means that $\Psi^*=a-bi$. Multiplying them together gives:

$$\begin{aligned}
\Psi\Psi^* &= (a+bi)(a-bi) && \text{Expand the brackets}\\
&= a^2+abi-abi-(bi)^2 && \text{Simplify this}\\
&= a^2-b^2i^2 && \text{Simplify the } i^2\\
&= a^2+b^2
\end{aligned}$$

Note: a^2+b^2 is also r^2 if the complex number was in polar or exponential form. Since r is called the modulus, $\Psi\Psi^*$ is often called the mod-squared distribution since it produces the modulus squared.

8 Matrices

8.1 What is a Matrix?

A matrix is defined as an array of numbers such as:

$$\begin{pmatrix} 3 & 1 & 8 \\ 0 & -4 & 5 \end{pmatrix}$$

- Matrices come in different sizes. We write the size of the matirx as rows $\times$ columns. So the matrix above is a 2×3 matrix.
- We use capital letters such as A or B to denote matrices.
- The numbers contained in a matrix are known as matrix elements. They are denoted a_{ij} where i represents the row and j the column in which the element is in. For example in the above matrix $a_{11} = 3$ and $a_{23} = 5$.
- Matrices with an equal number of rows and columns are called square matrices. For example the 2×2 matrix below:

$$\begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$$

Example: For the matrices below find the size of the matrix and the value of a_{21} and a_{33} if possible.

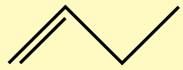
1. $A = \begin{pmatrix} 4 & 5 & 6 \\ 1 & 2 & 3 \\ 4 & 5 & 6 \\ 1 & 2 & 3 \end{pmatrix}$
2. $B = \begin{pmatrix} 1 \\ -1 \\ 40 \end{pmatrix}$
3. $C = \begin{pmatrix} a & b & c \\ e & d & f \\ g & h & i \end{pmatrix}$

Solution:

1. The matrix A has 4 rows and 3 columns, hence is a 4×3 matrix. We have that $a_{21} = 1$ and $a_{33} = 6$.
2. The matrix B has 3 rows and 1 column, hence is a 3×1 matrix. We have that $a_{21} = -1$ and a_{33} does not exist as this is a 3×1 matrix.
3. The matrix C has 3 rows and 3 columns, hence it is a 3×3 matrix (also a square matrix). We then have that $a_{21} = d$ and $a_{33} = i$

Matrices are an excellent way of expressing large amounts of information or data in a small space as shown in the next example.

Chemistry Example: Ignoring the hydrogens find the atom connectivity matrix of but-1-ene shown below:



Solution: An atom connectivity matrix describes how the carbons in but-1-ene are bonded with each other. First note that we have labelled the carbons 1-4. We use the matrix element a_{mn} (in row m and column n) to describe how carbon m and carbon n are bonded hence we need to find a 4×4 matrix.

- The matrix element a_{12} describes how carbon 1 is bonded to carbon 2, we have a double bond between them hence $a_{12} = 2$. This also means that $a_{21} = 2$ as this matrix element also describes how carbon 2 is bonded to carbon 1.
- The matrix element a_{13} describes how carbon 1 is bonded to carbon 3, we have no bond between them hence $a_{13} = 0$ this also means that $a_{31} = 0$.
- As there is a single bond between carbon 2 and carbon 3 we have $a_{23} = 1$ and $a_{32} = 1$
- The matrix element a_{11} describes how carbon 1 is bonded to carbon 1 however it does not make sense for an atom to be bonded to itself. Hence we tend to write in the atomic number of the atom which for carbon is 6 so $a_{11} = 6$. This is also true for $a_{22} = 6$, $a_{33} = 6$ and $a_{44} = 6$.

So when we find the rest of the matrix elements in the same way we have that the atom connectivity matrix of but-1-ene is:

$$\begin{pmatrix} 6 & 2 & 0 & 0 \\ 2 & 6 & 1 & 0 \\ 0 & 1 & 6 & 1 \\ 0 & 0 & 1 & 6 \end{pmatrix}$$

8.2 Matrix Algebra

Addition and Subtraction

Matrices can only be added or subtracted if they are of the same size. Suppose we have the 2×2 matrices below:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \text{ and } B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

Then their sum is found by adding together corresponding matrix elements:

$$\boxed{A + B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} + \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11} + b_{11} & a_{12} + b_{12} \\ a_{21} + b_{21} & a_{22} + b_{22} \end{pmatrix}}$$

Subtraction works in exactly the same way:

$$\boxed{A - B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} - \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11} - b_{11} & a_{12} - b_{12} \\ a_{21} - b_{21} & a_{22} - b_{22} \end{pmatrix}}$$

In general if we are adding or subtracting two $m \times n$ matrices:

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix} \pm \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{m1} & b_{m2} & \cdots & b_{mn} \end{pmatrix} = \begin{pmatrix} a_{11} \pm b_{11} & a_{12} \pm b_{12} & \cdots & a_{1n} \pm b_{1n} \\ a_{21} \pm b_{21} & a_{22} \pm b_{22} & \cdots & a_{2n} \pm b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} \pm b_{m1} & a_{m2} \pm b_{m2} & \cdots & a_{mn} \pm b_{mn} \end{pmatrix}$$

Note: Matrix addition and subtraction is commutative so $A + B = B + A$.

Example: Calculate the following:

1. $\begin{pmatrix} 1 & 1 \\ 4 & 0 \end{pmatrix} + \begin{pmatrix} -1 & 4 \\ 2 & -3 \end{pmatrix}$

2. $\begin{pmatrix} 10 \\ -3 \\ 0 \end{pmatrix} - \begin{pmatrix} -3 \\ 2 \\ 0 \end{pmatrix}$

3. $\begin{pmatrix} 9 \\ -2 \end{pmatrix} + \begin{pmatrix} -9 & 0 & 1 \\ 13 & 13 & 0 \\ 9 & 0 & 9 \end{pmatrix}$

Solution:

1. $\begin{pmatrix} 1 & 1 \\ 4 & 0 \end{pmatrix} + \begin{pmatrix} -1 & 4 \\ 2 & -3 \end{pmatrix} = \begin{pmatrix} 1 + (-1) & 1 + 4 \\ 4 + 2 & 0 + (-3) \end{pmatrix} = \begin{pmatrix} 0 & 5 \\ 6 & -3 \end{pmatrix}$

2. $\begin{pmatrix} 10 \\ -3 \\ 0 \end{pmatrix} - \begin{pmatrix} -3 \\ 2 \\ 0 \end{pmatrix} = \begin{pmatrix} 10 - (-3) \\ -3 - 2 \\ 0 - 0 \end{pmatrix} = \begin{pmatrix} 13 \\ -5 \\ 0 \end{pmatrix}$

3. We can not add these matrices as they are of different sizes!

Multiplication by a Constant

The simplest form of multiplication is where we multiply a matrix by a constant or scalar. We show the rule on a 2×2 matrix but it follows in the same way for any sized matrix we simply multiply every element by the scalar.

$$\boxed{\lambda A = \lambda \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \lambda a & \lambda b \\ \lambda c & \lambda d \end{pmatrix}}$$

Example: Find the following:

1. $2\begin{pmatrix} -1 & 2 \\ 0 & 4 \end{pmatrix}$
2. $\dfrac{\sqrt{3}}{3}\begin{pmatrix} -9 & 0 & 3 \\ 12 & 12 & 0 \\ 3 & 0 & 3 \end{pmatrix}$

Solution:

1. $2\begin{pmatrix} -1 & 2 \\ 0 & 4 \end{pmatrix} = \begin{pmatrix} -1 \times 2 & 2 \times 2 \\ 0 \times 2 & 4 \times 2 \end{pmatrix} = \begin{pmatrix} -2 & 4 \\ 0 & 8 \end{pmatrix}$
2. $\dfrac{\sqrt{3}}{3}\begin{pmatrix} -9 & 0 & 3 \\ 12 & 12 & 0 \\ 3 & 0 & 3 \end{pmatrix} = \begin{pmatrix} -9 \times \frac{\sqrt{3}}{3} & 0 \times \frac{\sqrt{3}}{3} & 3 \times \frac{\sqrt{3}}{3} \\ 12 \times \frac{\sqrt{3}}{3} & 12 \times \frac{\sqrt{3}}{3} & 0 \times \frac{\sqrt{3}}{3} \\ 3 \times \frac{\sqrt{3}}{3} & 0 \times \frac{\sqrt{3}}{3} & 3 \times \frac{\sqrt{3}}{3} \end{pmatrix} = \begin{pmatrix} -3\sqrt{3} & 0 & \sqrt{3} \\ 4\sqrt{3} & 4\sqrt{3} & 0 \\ \sqrt{3} & 0 & \sqrt{3} \end{pmatrix}$

Matrix Multiplication

Suppose we want to find the product AB of the matrices A and B. Then:

- The number of columns of A must be equal to the number of rows of B.
- The product matrix has the same number of rows as A and the same number of columns as B.

Below we have the rule for find the product of two 2×2 matrices:

$$\boxed{AB = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix}}$$

In general if we want to find the product AB of a $m \times l$ matrix A and $k \times n$ matrix B:

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1l} \\ a_{21} & a_{22} & \cdots & a_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{ml} \end{pmatrix} \text{ and } B = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{k1} & b_{k2} & \cdots & b_{kn} \end{pmatrix}$$

$$\text{so that } AB = \begin{pmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mn} \end{pmatrix}$$

IMPORTANT: We calculate c_{ij} to be the scalar dot product of row i and column j.

Example: Find the following products:

1. $\begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} 3 & 1 \\ 2 & 1 \end{pmatrix}$
2. $\begin{pmatrix} 10 & 2 & 2 \\ 8 & -1 & 4 \end{pmatrix}\begin{pmatrix} -5 & -3 \\ 2 & 2 \end{pmatrix}$

Solution:

1. As we are multiplying a 2×2 matrix by another 2×2 matrix the product matrix will also be a 2×2 matrix in the form below:

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

We now calculate the elements of the product matrix above:

To find a_{11} we take the dot product of row 1 and column 1:

$$a_{11} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \bullet \begin{pmatrix} 3 \\ 2 \end{pmatrix} = 1 \times 3 + 0 \times 2 = 3$$

To find a_{12} we take the dot product of row 1 and column 2:

$$a_{12} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \bullet \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 1 \times 1 + 0 \times 1 = 1$$

To find a_{21} we take the dot product of row 2 and column 1:

$$a_{21} = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \bullet \begin{pmatrix} 3 \\ 2 \end{pmatrix} = 2 \times 3 + 1 \times 2 = 8$$

To find a_{22} we take the dot product of row 2 and column 2:

$$a_{22} = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \bullet \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 2 \times 1 + 1 \times 1 = 3$$

$$\begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} 3 & 1 \\ 2 & 1 \end{pmatrix} = \begin{pmatrix} 3 & 1 \\ 8 & 3 \end{pmatrix}$$

2. The number of columns of the matrix on the left does not equal to the number of rows of the matrix on the right hence this product can not be found!

Note: Matrix multiplication is **NOT** commutative so $AB \neq BA$

Example:

Let $A = \begin{pmatrix} 1 & 1 \\ 4 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} -1 & 4 \\ 2 & -3 \end{pmatrix}$

Then $AB = \begin{pmatrix} 1 & 1 \\ -4 & 16 \end{pmatrix}$ and $BA = \begin{pmatrix} 15 & -1 \\ -10 & 2 \end{pmatrix}$

This shows that matrix multiplication is not commutative as $AB \neq BA$.

8.3 The Identity Matrix, Determinant and Inverse of a Matrix

The Identity Matrix

The Identity Matrix (or Unit Matrix) is a square matrix which is denoted I and has '1' along the leading diagonal (from top left to bottom right) with '0' in all other positions.

The 2×2 identity matrix is:

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The 3×3 identity matrix is:

$$I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

In general the $n \times n$ identity matrix is:

$$I_n = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

The Identity matrix has the property that when multiplied with another matrix it leaves the other matrix unchanged:

$$\boxed{AI = A = IA}$$

Example:

$$\begin{pmatrix} 3 & 4 \\ 8 & 9 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 3 & 4 \\ 8 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 3 & 4 \\ 8 & 9 \end{pmatrix}$$

The Transpose of a Matrix

The transpose of a matrix is denoted A^T and is obtained by interchanging the rows and columns of the matrix. The rule for a 2×2 matrix A is:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$A^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

Note: There exists a more complex formula for 3×3 matrices.

Example: For the matrix A below find A^T.

$$A = \begin{pmatrix} 3 & 4 \\ 8 & 9 \end{pmatrix}$$

Solution:

$$A^{-T} = \begin{pmatrix} 3 & 8 \\ 4 & 9 \end{pmatrix}$$

The Determinant of a Matrix

The determinant of a matrix is denoted $|A|$. For finding the determinant of a 2×2 matrix A we have the following formula:

$$\boxed{\text{For } A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \text{ the determinant is } |A| = ad - bc}$$

Note: There exists a more complex formula for finding the determinants of 3×3 matrices.

- A matrix whose determinant is zero so $|A| = 0$ is said to be singular.
- A matrix whose determinant is non zero so $|A| \neq 0$ is said to be non-singular.

Example: Find the determinant of the matrix A:

$$A = \begin{pmatrix} 1 & -4 \\ 2 & 5 \end{pmatrix}$$

Solution:

$$|A| = \begin{vmatrix} 1 & -4 \\ 2 & 5 \end{vmatrix} = (1 \times 5) - (-4 \times 2) = 13$$

Note: The matrix A is non-singular.

Inverse of a Matrix

Only non-singular matrices have an inverse matrix. The inverse of a matrix A is denoted A^{-1} and has the following property:

$$\boxed{AA^{-1} = A^{-1}A = I}$$

To find the inverse of a 2×2 matrix A we have the following formula:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad A^{-1} = \frac{1}{|A|}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

$$\text{where } |A| = ad - bc \neq 0$$

Note: There exists a more complex formula for finding the inverses of 3×3 matrices.

Example: Find the inverse A^{-1} of the matrix A.

$$A = \begin{pmatrix} 1 & -4 \\ 2 & 5 \end{pmatrix}$$

Solution: From the previous example on determinants we know that $|A| = 13$. So the inverse of A is:

$$A^{-1} = \frac{1}{13}\begin{pmatrix} 5 & 4 \\ -2 & 1 \end{pmatrix} = \begin{pmatrix} \frac{5}{13} & \frac{4}{13} \\ -\frac{2}{13} & \frac{1}{13} \end{pmatrix}$$