CH10009 Workshop Questions

Fiona Dickinson

2021-07-20

Contents

Welcome

The notes have been prepared in a package called BookDown for RStudio so that the equations are accessible to screen readers. However, by providing the notes as a .html webpage I can also embed short videos to further describe some of the topics. Further you can download the questions (and later the answers, top left of the screen) in a format that suits you (either pdf or epub) to view offline, or change the way this document appears for ease of reading.

If you spot any typos or think there are any errors please let me know and I will do my best to fix them.

Workshops for CH10009

The topics for LOILS each week are as follows:

- Week 1: General Q&A
- Week 2: Rearranging equations, units and standard form
- Week 3: Logarithms and exponentials
- Week 4: Tables and graphs
- Week 5: Calculus - differentiation - the basics and the chain rule
- Week 6: Calculus - differentiation - the product rule and partial differentiation
- Week 7: Calculus - integration - the basics and definite integrals
- Week 8: Some more examples of integration and revision

This 'book' will be updated weekly with workshop questions, answers will be provided and some answers will include 'process' as well as answer. Please contact me if you need help.

I am using this format as it is an accessible format.

Version history

Version 1.1 in progress July 2021.

Version 1.0 complete December 2020.

The initial commit of this book is dated 2nd October 2020.

Chapter 1

Week 1 - Rearranging equations and units

1.1 Preliminary infomation

This workshop contains some fundamental materials on both rearranging equations and units. Unfortunately both of these things result in lost marks for a number of candidates either because of carelessness or lack of understanding.

Bad habits in rearranging equations, such as trying to undertake too many steps at once often lead to error, mantras such as 'change the side change the sign' are often an oversimplification and may lead to error.

Values have to have units, without them things make no sense, and in science we cannot assume units on context. Converting between units is equally important and famously errors can occur. You should 'work out' your unit in every case, not just assume it is something and writing that down.

In short, show your working clearly, if you do so you *will* make fewer mistakes. Paper doesn't cost much, and if you write on a tablet each new page is free so please space out your work, when learning things annotate your work with useful things (this will help you revise), and make it clear!

1.1.1 Rearranging equations

'Change the side change the sign' is often running through peoples' heads as they rearrange equations, however it is only of limited utility as it makes no sense when considering logs or exponentials. More correctly we should think about using reciprical functions on both sides of an equation, for example if I multiply both sides of an equation by the same thing it is mathematically equivalent of doing nothing.

This subtle distinction would 'fix' almost all of the common errors seen in chemistry.

If we start with one of the most important equations in chemistry, the Gibbs' equation:

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

Here the capital 'delta' (Δ) in each case means 'large change in' and so they cannot be canceled.

If I wanted to rearrange this equation to make ΔS, the entropy change, the subject then:

Start by adding $T\Delta S$ to both sides of the equation:

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

on the right hand side $-T\Delta S + T\Delta S = 0$ and so cancel.

We can then subtract ΔG from both sides of the equation:

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

now the $\Delta G - \Delta G$ on the left hand side of the equation cancel, leaving us with:

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

Now to cancel the 'T' on the left hand side we need to divide by 'T' on both sides:

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

which leaves us with an equation with ΔS as the subject:

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

I recognise as show this is extreamly arduous, however it is changing how we think about the problem which is important.

1.1.2   SI base units

Despite cultural tendancies to hold onto older units (such as pounds & ounces, calories, Calories and miles) in science all units are directly derived from the international standard SI system.

Althought there have been many versions of metric units over the years it became increasingly important to standardise units. The SI system of base units

has seven fundamental units (Table 1.1) from which all other units are derived. Recently there has been interest in finding more fundamental ways to describe each of these units (rather than an actual lump (mass) or bar (length) of platinum) whereby units are described by relation to physical constants (such as the speed of light, or Avagadro's constant which define the meter and mole respectively).

Table 1.1: The seven base units from which all others are dervied.

SI base unit	symbol	quantity symbol (dimension)	quantity
kilogram	kg	M	mass
metre	m	L	length
second	s	T	time
ampere	A	I	electric current
kelvin	K	Θ	temperature
mole	mol	N	amount of substance
candela	cd	J	luminous intensity

1.1.3 SI Derived units

James Clarke Maxwell developed the field of dimensional analysis. Dimensional analysis shows that units have to be consistent in equations.

To add to values in an equation they must have the same unit - so I can't add kJ mol^{-1} to J K^{-1} mol^{-1}, nor can I directly add kJ mol^{-1} to J mol^{-1}.

When multiplying or dividing values with units then the units combine (by performing the same operation). Velocity is displacment (in m) divided by time (in s), and so the unit of velocity is m s^{-1}.

Some 'combined units' have been given their own unique names (Table 1.2), these often make it easier to use the unit (it is a lot easier to say 'volt' than kg m^2 s^{-3} A^{-1} each time you need to use it). The case of these units (just as with the SI base units) is important, however it should be noted when writing the unit name, even if they are named for a person, that name begins with a lower case letter.

Table 1.2: Some common named SI derived units used in chemistry.

symbol	SI derived unit	quantity	SI base units	other SI units
Hz	hertz	frequency	s^{-1}	
N	newton	force	kg m s^{-2}	
Pa	pascal	pressure	kg m^{-1} s^{-2}	N m^{-2}
J	joule	energy	kg m^2 s^{-2}	N m
W	watt	power	kg m^2 s^{-3}	J s^{-1}
C	coulomb	electrical charge	A s	

symbol	SI derived unit	quantity	SI base units	other SI units
V	volt	electrical potential	$kg\ m^2\ s^{-3}\ A^{-1}$	$J\ C^{-1}$
F	farad	electrical capacitance	$kg^{-1}\ m^{-2}\ s^4\ A^2$	$C\ V^{-1}$
Ω	ohm	electrical resistance	$kg\ m^2\ s^{-3}\ A^{-2}$	$V\ A^{-1}$
S	siemens	electrical conductance	$kg^{-1}\ m^{-2}\ s^3\ A^2$	$A\ V^{-1}$ or $1/\Omega$

Having said that, Table 1.2 contains some common units used in chemistry the units most used in chemistry for concentration, thermodynamics and kinetics are so far not named for anyone and so are usually written in full form. However mol dm^{-3} is often shortend to M (for molarity), this is a unit I use a lot and so in many questions you will see concentrations given as (for example) 0.250 mM or 1.000 M (not the longer 0.250 mmol dm^{-3} or 1.000 mol dm^{-3}).

Please note when reporting compound units there should be a space between each unit, so it is $J\ K^{-1}\ mol^{-1}$ not $JK^{-1}mol^{-1}$.

1.1.4   Other units and conversion factors

There are a number of non-SI base or derived units which are in common usage which are useful to know and be able to convert between. Table 1.3 contains a number of useful unit conversions.

Table 1.3: The relationship between some other common units and the SI system.

unit	quantity	SI equivalant
torr (or mm Hg)	pressure	$\frac{101325}{760}$ Pa
atm	pressure	101325 Pa
bar	pressure	100000 Pa
eV	energy	$1.602176634 \times 10^{-19}$ J
cal	energy	4.184 J
Cal	energy	4.184 kJ
Å	length	1×10^{-10} m

There are myriad other units in use, either with historical or geographic preference, or just for niche purposes (where would we be without olympic swimming pools or London buses). Examples such as the mile, furlong or beard-second are all units of length.

Further, the unit ºC is formally an SI derived unit. The temperature in kelvin is:

$$T(\text{K}) = T(^{\circ}\text{C}) + 273.15$$

Just a note to say that this 273.15 K conversion is 'precise' in other words we can consider it to have infinite significant figures, and so if we happen to know temperatures in centigrade to more than two decimal places we do not loose any of these in conversion to kelvin.

1.1.5 SI prefixes and standard form

In general lower case prefixes are used for negative powers and upper case prefixes are used for positive powers, however k (kilo) is an obvious exception to this rule. (Other exceptions are da (deca, 10^1) and h (hecto, 10^2)).

Table 1.4: The more common SI prefixes used in chemistry.

SI prefix	SI prefix 'name'	standard form multiplier
y	yocto	10^{-24}
z	zepto	10^{-21}
a	atto	10^{-18}
f	femto	10^{-15}
p	pico	10^{-12}
n	nano	10^{-9}
	micro	10^{-6}
m	milli	10^{-3}
c	centi	10^{-2}
d	deci	10^{-1}
k	kilo	10^3

When prefixes are used there is no space between prefix and unit, (so mm (millimeter) not m m (which could be confused for meter meter)).

There can be some confusion with prefixes and inverse units, for example ns^{-1} is the same unit as 1/ns. This could be more properly written as 10^9 s^{-1} (and is not in fact 10^{-9} s^{-1}).

When there are squares (or cubes) combined with prefixes it is a statement that the prefix is squared (or cubed) as well. So for example 1 cm^2 is quite literally 1 cm $\times$ 1 cm (or 1 $\times$ 10^{-4} m^2).

1.2 Examples

1.2.1 Conversion of mL to L or cm^3 to dm^3

One of the most common conversions undertaken in the physical chemistry lab is conversion of mL to L (or more correctly cm^3 to dm^3), and although most

people are happy to know 'you just divide by 1000' most haven't thought 'why', nor does everyone get this unit conversion correct.

Both of these examples are shown in a worked video at teh end of this section, as is a pdf of the handwritten notes from this video.

1.2.1.1   Conversion of mL to L

We can solve this logially, by first having the assertion that $1 \text{ mL} = 1 \times 10^{-3}$ L. Therefore when I want to convert mL to L I just multiply by 1×10^-3 (which is equivalent to dividing by 1000), or more formally:

$1 \text{ mL} = 1 \times 10^{-3}$ L

$1 = 1 \times 10^{-3}$ L mL^{-1}

anything may be multiplied by 1 and there be no change and so if I were to want to convert 27.2 mL to L then:

$27.2 \text{ mL} \times 1 \times 10^{-3}$ L mL^{-1}

we can see that the units of mL and mL^{-1} cancel and we are left with just L and so:

$27.2 \text{ mL} = 27.2 \times 10^{-3}$ L

Writing this as either 27.2×10^{-3} L or 0.0272 L are both equivalent and both valid.

1.2.1.2   Conversion of cm^3 to dm^3

It will come as no surprise to know that the same process of either multiplying by 1×10^{-3} or dividing by 1000 will correctly do this conversion, however knowing that can help justify the process here.

I am going to start with a similar assertion as above:

$1 \text{ cm} = 1 \times 10^{-2}$ m

and so

$1 \text{ cm}^3 = (1 \times 10^{-2})^3 \text{ m}^3 = 1 \times 10^{-6} \text{ m}^3$

and equivalently

$1 \text{ dm} = 1 \times 10^{-1}$ m

(remember the prefix is raised to the same power as the number) and so:

$1 \text{ dm}^3 = (1 \times 10^{-1})^3 \text{ m}^3 = 1 \times 10^{-3} \text{ m}^3$

for each of these I can make statements where 1 equals something...

$1 = 1 \times 10^{-6} \text{ m}^3 \text{ cm}^{-3}$

$1 = 1 \times 10^{-3} \text{ m}^3 \text{ dm}^{-3}$

and I can then combine these into a single statement by dividing one by the other:

$1 = 1 \times 10^{-6}$ m^3 cm^{-3} / 1×10^{-3} m^3 dm^{-3}

which simplifies (because m^3 cancels and so do some of the powers of 10) to :

$1 = 1 \times 10^{-3}$ dm^3 cm^{-3}

again if we take the example of 27.2 cm^3 (which is the more formal unit of mL) then:

27.2 cm^3 = 27.2 cm^3 $\times$ 1×10^{-3} dm^3 cm^{-3} = 27.2×10^{-3} dm^3

Now I have broken both of these down into multiple steps, and it is good to do this until you become more confident in these conversions, but in time you will be able to streamline this process.

This video shows me working through both of the above problems:

The 'notes' from this video may be found here.

1.3 Questions

1.3.1 Rearranging equations

Answers for these questions are in Section 1.4.1.

For each of the following rearrange to make the specified variable the subject of the equation.

1. $[A] = [A]_0 - kt$, t
2. $E = \frac{1}{2}mv^2$, v
3. $F = \frac{q_1 q_2}{4\pi\varepsilon_0 r^2}$, r
4. $\frac{1}{[A]} = \frac{1}{[A]_0} + kt$, $[A]_0$
5. $\ln(x_A) = -\frac{\Delta H}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$, T_1
6. $K_a = \frac{\alpha^2 c}{1-\alpha}$, α

1.3.2 Unit conversion questions

Answers for these questions are in Section 1.4.2.

1. Convert the following:
   a. 3.4 µm to mm and m
   b. 270.4 g mol^{-1} to kg mol^{-1} and yg (molecule^{-1})
   c. 23.4 g dm^{-3} to mg dm^{-3}, g m^{-3}, and kg m^{-3}
   d. 17.5 µHz to Hz
   e. 5796 cm^{-1} to µm^{-1} and m^{-1}

2. If a box has dimensions 0.234 m x 34.5 cm x 26.8 mm. What is the volume of the box in:
   a. cm^3?
   b. dm^3?
   c. m^3?
   d. $Å^3$?

---

3. The Gibbs free energy of a reaction, ΔG is given by equation (1.1).

$$\Delta G = \Delta H - T\Delta S \tag{1.1}$$

Determine the value of ΔG at 40 ºC when the enthalpy of reaction, $\Delta H = $ -10.235 kJ mol⁻¹ and the molar entropy, $\Delta S = $ +34 J K⁻¹ mol⁻¹

1.3.3   Determining units of variables in equations

Answers for these questions are in Section 1.4.3.

1. The ideal gas equation is given in equation (1.2).

$$pV = n\mathrm{R}T \tag{1.2}$$

The units of the variables are: p (pressure), Pa (pascals) V (volume), m^3 n (number of moles), mol T (absolute temperature), K

   a. Determine the SI base units of the gas constant, R.

   b. Determine the pressure in mmHg of 1.00 mmol of an ideal gas that occupies 1.65 dm^3 at 25 ºC.

---

2. The famous Einstein equation $E = mc^2$ is more properly written as:

$$E^2 = p^2c^2 + m_0^2c^4$$

Determine the units of the variable p.

---

3. At low temperatures the molar heat capacity of a material $C_{p,m}$ (J K⁻¹ mol⁻¹) is given by equation (1.3).

$$C_{p,m} = aT^3 \tag{1.3}$$

Determine the units of the constant, a.

4. Determine the units of the coulomb constant, k_e, in equation (1.4), given that r is the separation of two charges, F the force of attraction between the two charges, and q_x is the charge (in coulombs, C) on each of the particles.

$$F = k_e \frac{q_1 q_2}{r^2} \tag{1.4}$$

1.4 Answers

Where available videos of worked examples are shown in hyperlinks with each answer.

1.4.1 Rearranging equations answers

1. $t = \frac{[A]_0 - [A]}{k}$

2. $v = \sqrt{\frac{2E}{m}}$

3. $r = \sqrt{\frac{q_1 q_2}{4\pi\varepsilon_0 F}}$

4. $[A]_0 = \frac{[A]}{1 - [A]kt}$

5. $\frac{\Delta H T_2}{\Delta H - RT \ln x_A}$ Worked answer

6. $\alpha = \frac{-K_a \pm \sqrt{K_a^2 + 4cK_a}}{2c}$ Worked answer

1.4.2 Unit conversion answers

1. a. 3.4×10^{-3} mm; 3.4×10^{-6} m
    b. 0.2704 kg mol^{-1}; 449.0 yg
    c. 23.4×10^{-3} mg dm^{-3}; 23.4×10^{-3} g m^{-3}; and 23.4×10^{-6} kg m^{-3}
    d. 17.5×10^{-6} Hz
    e. 0.5796 µm^{-1} and 5.796×10^5 m^{-1}

2. a. 2.16×10^3 cm^3
    b. 2.16 dm^3
    c. 2.16×10^{-3} m^3
    d. 2.16×10^{27} Å^3

3. -21 kJ mol^{-1} - please note this value is correct to the appropriate sig figs

1.4.3   Determining units of variables in equations answers

1. a. • kg m^2 s^{-2} K^{-1} mol^{-1} (this is more ususally written as J K^{-1} mol^{-1})

    b. • 11.3 mm Hg (1.50 kPa)

    _____

2. kg m s^{-1}

    _____

3. J K^{-4} mol^{-1}

    _____

4. kg m^3 s^{-4} A^{-2} or N m^2 C^{-2}

Chapter 2

Week 2

2.1 Preliminary infomation

2.1.1 Rules of powers and exponents

$$m^a \times m^b = m^{a+b} \tag{2.1}$$

$$\frac{p^a}{p^b} = p^{a-b} \tag{2.2}$$

$$\left(q^a\right)^b = q^{a \times b} \tag{2.3}$$

Anything raised to the power 0 is equal to 1.

$$x^0 = 1$$

Roots may be expressed as fractional powers:

$$\sqrt[n]{x} = x^{\frac{1}{n}} \tag{2.4}$$

When we see negative powers it is the same as the inverser of the positive power.

$$x^{-n} = x^{\frac{1}{x^n}} \tag{2.5}$$

2.1.2   Rules of logs

Logs are the inverse function of exponents, and can have many bases:

When we use 'natural logs' we use the terminology ln, a natural log is the inverse of 'e'.

$$x = \ln e^x \tag{2.6}$$

Other logs are ususally marked with the *base*, however if no base is indicated it should be considered that this is $\log_{10}$.

$$x = \log_{10} 10^x \tag{2.7}$$

When combining logs (these rules are the same regardless of base):

$$\log_x A + \log_x B = \log_x(AB) \tag{2.8}$$

$$\log_x A - \log_x B = \log_x\left(\frac{A}{B}\right) \tag{2.9}$$

$$\log_x(A^n) = n \log_x A \tag{2.10}$$

If we want to change the bases of logs (such as in the Beer-Lambert law):

$$log_b A = \frac{\log_x A}{\log_x b} \tag{2.11}$$

2.2   Questions

2.2.1   Simple log practice

Answers for these questions are in Section 2.3.1.

Evaluate the following expressions:

1. $\log_{10} 10^6$
2. $\log_{10} 10^{-5}$
3. $\log_{10}(5^4 \times 3^{-2})$
4. $\ln \pi 6^2$
5. $e^{\log_e x} = \ln y$

2.2.2 Rearranging equations

Answers for these questions are in Section 2.3.2

1. Rearrange the following to make the highlighted term the subject:
   a. $\Delta S = k_B \ln W$, W
   b. $\Delta S = nR \ln \frac{V_f}{V_i}$, V_f
   c. $\nu = \frac{1}{2\pi} \left(\frac{k}{\mu} \right)^{\frac{1}{2}}$, μ
   d. $\ln K = \frac{nFE}{RT}$, E
   e. $\ln K' - \ln K = \frac{\Delta H}{R} \left(\frac{1}{T} - \frac{1}{T'} \right)$, ΔH

   ---

2. The integrated rate equation for a first order reaction is $[A] = [A]_0 e^{-kt}$.
   a. Rearrange this equation in order to make k the subject.
   b. What units must k have?

2.2.3 pH question.

Answers for these questions are in Section 2.3.3

HCl fully dissociates in water. If 5 cm^3 (measured using a glass pipette) of 38% w/w HCl solution ($\rho = 1.189$ kg dm^{-3}) is 'added to 20 cm^3 water'made up' in a 25 cm^3 standard flask.

   a. What is the pH of the resulting solution?
   b. What mass of NaOH is required to neutralise the resulting solution?

Hint: w/w means weight-weight, i.e. the number of g in 100 g. In this case 38 g of HCl in 100 g total of mixture.

Hint: you will need to think about units and rearranging equations from Week 1.

2.2.4 pK$_a$ question.

Answers for these questions are in Section 2.3.4

The degree of dissociation of an acid, α is related to the acid dissociation constant, K_a and the concentration of the acid, c, as shown in equation (2.12)

$$K_a = \frac{\alpha^2 c}{1 - \alpha} \tag{2.12}$$

Determine the pH of hydrofluoric acid solutions (pK_a = 3.18) when the concentration of acid is:

   a. 1.00 M
   b. 2.50 mM

Hint: We rearranged this equation last week for α

2.3   Answers

2.3.1   Simple log practice answers

1. 6
2. -5
3. 1.841...
4. 4.728...
5. $x = \ln y$

2.3.2   Rearranging equations answers

1. Rearrange the following to make the highlighted term the subject:

    a. $W = e^{\frac{\Delta S}{k_B}}$

    b. $V_f = V_i e^{\frac{\Delta S}{nR}}$

    c. $\mu = \frac{1}{4\pi^2} \frac{k}{\nu^2}$

    d. $E = \frac{RT}{nF} \ln K$

    e. $\Delta H = \left(\frac{TT'}{T'-T} \right) R \ln \frac{K'}{K}$

    _____

2.   a. $k = \frac{\ln[A]_0 - \ln[A]}{t}$

      b. s^{-1}

2.3.3   pH answer

a. pH -0.394

b. $m_{\text{NaOH}} = 2.5$ g

2.3.4   pK$_a$ answer

a. Two roots: 0.025 and -0.026 and we can't have a negative degree of dissociation. pH 1.6

b. Two roots: 0.40 and -0.66 and we can't have a negative degree of dissociation. pH 3.0

Chapter 3

Week 3

3.1 Preliminary infomation

3.1.1 Presentation of units on tables and graphs

Your tables should have units expressed in the column headers where appropriate, and uncertainties should be expressed in the header if they are constant across the whole range, or in parentheses for each measurement if different. Units should be expressed as "Quantity / unit" to allow you to express them as dimensionless quantities in the table or on the axis of your graph (please note brackets are absolutely incorrect).

This is because this is how our governing body (IUPAC) tell us how to do it. See the IUPAC Green Book (2012 edition, page 3).

You can think of the horizontal line below the header as an equals sign, so:

Table 3.1: The effect of potassium iodide concentration on emission intensity and fluorescence lifetime of acridone in aqueous solution.

[KI] / M	[KNO$_2$] / M	Emission intensity / 10^3 cps	/ ns
0	1.100	16.580	17.60
0.040	1.060	3.753	3.90
0.100	1.000	1.566	1.80
0.200	0.900	0.721	0.95
0.300	0.800	0.446	0.64
0.500	0.600	0.242	0.39
0.800	0.300	0.121	0.25

in the table above the third value down in the first column can be expressed as:

[KI] / M = 0.100

which of course rearranges to:

[KI] = 0.100 M.

If we look at the top value in the third column:

Emission intensity / 10^3 cps = 16.580

which of course rearranges to:

Emission intensity = 16.580 × 10^3 cps

3.1.2   Plotting of graphs

When ever we plot a graph we have to determine what we plot on each of the two axes.

The independent variable is the variable we have control over, we plot it (or something related to it) on the x-axis (the horizontal axis).

The dependent variable is the varible we measure, we plot it (or something related to it) on the y-axis (the vertical axis).

These axis should under most circumstances not contain constants unless those constants are specific to the experiment.

There is no need to start a graph axis at zero - you do not need a 'squiggle' on the axis to show that it is not starting at zero (that is what the numbers on the axis tell you), this squiggle (or more formally an axis break) does have a job when plotting graphs, but usually the use by first year undergraduates is incorrect.

When plotting a graph, we want to have broken down the equation we are using to fit the linear relationship:

$$y = mx + c \tag{3.1}$$

We should never force a graph through a particular intercept (c).

It is important when we ever have performed a calculation to determine values to plot on either x or y axis that we have taken account for any multipliers in the header, and that units ar SI (such as tempeature in K!).

A gradient is calculated by determining the change in y divided by the change in x:

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

Don't forget units on gradients! The units of a gradient are the units on y divided by the units on x.

3.1.3   Example of plotting graphs

The Stern-Volmer (Equation (3.4)) shows how the lifetime τ of a dye changes with concentration of a quencher, [Q]. The data in Table 3.1 can be modeled using the Stern-Volmer equation, you will note that this equation uses terms with a subscript 0 (τ_0), when values like this are frequently used in chemistry (and physics).

$$\frac{\tau_0}{\tau} = 1 + k[Q] \tag{3.2}$$

where $k = k_q \tau_0$.

These 'subscript 0' values are referencing values when the independant variable is zero, so $\tau_0 = 17.60$ ns.

You will notice that Equation (3.4) is already arranged into $y = mx + c$, where the x variable is [KI] and the y variable is $\frac{\tau_0}{\tau}$. This means that the gradient is k, and the intercept 1.

3.2   Questions

When plotting graphs feel free to plot either by hand, in python, excel or numbers. The choice is entirely up to you.

3.2.1   Sketch graphs

Answers for these questions are in Section 3.3.1.

For the following equations sketch suitable linear plots indicating values of the intercept and gradient on each sketch.

1. Show how absorption, A, changes with concentration, c: $A = \varepsilon cl$

2. Show how pressure, p, changes with temperature, T: $pV = nRT$

3. Show how pressure, p, changes with volume, V: $pV = nRT$

3.2.2   Second order kinetics

Answers for these questions are in Section 3.3.2.

Use the following table of data to plot a graph of $\frac{1}{[A]}$ against t. Find the gradient and intercept.

(Just to note here you are plotting the equation $\frac{1}{[A]} = \frac{1}{[A]_0} + kt$).

t / s	10^4 [A] / mol dm^{-3}
100	21.0

t / s	10^4 [A] / mol dm^{-3}
200	12.0
300	8.4
400	7.1
500	5.6

3.2.3   Clausius-Clapeyron equation

Answers for these questions are in Section 3.3.4.

The relationship between the vapour pressure and temperature of diethyl ether (Table 3.3) can be modeled using the Clausius-Claeyron equation (Equation (3.3)) to determine the enthalpy of vapourisation $\Delta_{vap}H^\circ$.

$$\ln p = -\frac{\Delta_{vap}H^\circ}{RT} + C \tag{3.3}$$

1. Determine $\Delta_{vap}H^\circ$.
2. Determine the temperature diethyl ether boils at, at 1 atmosphere (760 mm Hg). *Hint: determine C*

Table 3.3: The measured vapor pressure of ether (in mm Hg) at sub-zero temperatures.

p / mm Hg	T / °C
17	-38
28	-30
40	-25
55	-20
75	-15
97	-10
125	-5
157	0

3.2.4   Arrhenius equation

Answers for these questions are in Section 3.3.4.

The Arrhenius equation (Equation (3.4) shows how the rate of reaction, k, depends upon the temperature of the reaction, T).

$$k = Ae^{-\frac{E_a}{RT}} \tag{3.4}$$

For the data shown in Table 3.4 plot an appropriate linear plot in order to

determine the activation energy, E_a, and the pre-exponential factor, A.

Table 3.4: The variation of measured rate constant with temperature for an undergraduate's experiment.

T / °C	k / 10^5 s^{-1}
283	0.000352
356	0.0302
393	0.219
427	1.16
508	39.5

3.3   Answers
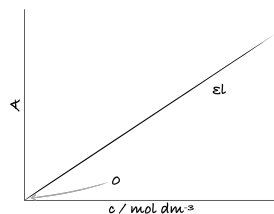
3.3.1   Sketch graphs

1.

Figure 3.1: The Beer-Lambert relationship to show how absorbance, the dependent variable, changes with concentration, the independent variable.
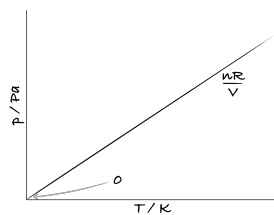
2.

Figure 3.2: A sketch to show how the pressure of an ideal gas, the dependent variable,changes with temperature, the independent variable.

3.
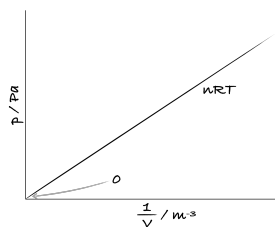
Figure 3.3: A sketch to show how the pressure of an ideal gas, the dependent variable,changes with volume, the independent variable - note for a linear relationship we have 1/V on the x-axis.

3.3.2   Second order kinetics

m = 3.19 M^{-1} s^{-1}, c = 180 M^{-1} ([A]$_0$ = 5.56 mM)

3.3.3   Clausius-Clapeyron equation

$\Delta_{vap}H°$ = 31.6 kJ mol^{-1}, 39 ºC.

3.3.4   Arrhenius equation

m = -22.4 × 10^3 K, c = 43.7, E_a = 186 kJ mol^{-1}, A = 9.7 × 10^{18} s^-1

Chapter 4

Week 4

4.1 Preliminary infomation

$f(x) \equiv y$	$f'(x) \equiv \dfrac{\mathrm{d}y}{\mathrm{d}x}$
A	0
Ax^n	nAx^{n-1}
$\dfrac{A}{x^n} \equiv Ax^{-n}$	$-nAx^{-n-1}$
e^{Ax}	Ae^{Ax}
$A\ln Bx$	$\dfrac{A}{x}$
$\sin Ax$	$A\cos Ax$
$\cos Ax$	$-A\sin Ax$
$\tan Ax$	$-A\sec^2 Ax$
$Au + Bv$	$A\dfrac{\mathrm{d}u}{\mathrm{d}x} + B\dfrac{\mathrm{d}v}{\mathrm{d}x}$

Chain Rule:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}y}{\mathrm{d}u} \times \frac{\mathrm{d}u}{\mathrm{d}x}$$

4.2 Questions

4.2.1 'Simple' differentiation

1. Find $\dfrac{\mathrm{d}y}{\mathrm{d}x}$ of the following functions:

a. $y = 6x + 4$
b. $y = 5x^2 + 3x - 7$

c. $y = x^{-\frac{1}{2}} + 3x - 4$

d. $6x^{\frac{2}{3}} - x + 9$

2. Find $\dfrac{\mathrm{d}y}{\mathrm{d}x}$ of the following functions:

a. $y = 3x^2 + \cos x$

b. $y = 6\ln 2x$

c. $y = \frac{2}{3}e^{\frac{3x}{2}}$

d. $y = -e^{-5x} - e^{5x}$

4.2.2   Turning points

Find the turning points (x, y) for the following functions:

1. $y = 2x^3 - 9x^2 + 12x$

2. $y = 12x^5 - 45x^4 + 40x^3$

4.2.3   Chain rule

Find the turning points (x, y) for the following functions:

1. $y = sin^2(x)$

2. $y = sin(e^{4x})$

3. $y = e^{(7x^2 + 2x)}$

4. $y = (x - 1)^9$

4.2.4   Applied questions

1. If two electric dipoles are aligned in an adjacent parallel manner such that they are separated by distance r, their potential energy of interaction, V, is given by:

$$V = \frac{\mu_1 \mu_2}{4\pi\varepsilon_0 r^3}$$

determine $\dfrac{\mathrm{d}V}{\mathrm{d}r}$

2. Light is scattered as it passes though solutions containing small particles with an intensity I, given by the following expression:

$$I = I_0 \frac{\pi\alpha^2}{\varepsilon_r^2 \lambda^4 r^2})(\sin\phi)^2$$

determine expressions for how the intensity varies with:

a. wavelength,

b. angle,

c. distance from scatterer, r

formally these are partial derivatives and we will learn about them next week

3. The radius of a spherical balloon is increasing at a rate of 0.2 m s^{-1}. Find the rate of increase of (a) the volume and (b) the surface area of the balloon at the instant when the radius is 1.6 m.

4.3 Answers

4.3.1 'Simple' differentiation

1. $\dfrac{\mathrm{d}y}{\mathrm{d}x} =$

a. 6
b. $10x + 3$
c. $-\frac{1}{2}x - \frac{3}{2} + 3$
d. $4x^{-\frac{1}{3}} - 1$

2. $\dfrac{\mathrm{d}y}{\mathrm{d}x} =$

a. $6x - \sin x$
b. $\frac{6}{x}$
c. $e^{\frac{3x}{2}}$
d. $5e^{-5x} - 5e^{5x}$

4.3.2 Turning points

1. $(1,5)$max, $(2,4)$min
2. $(0,0)$ POI$(+/+)$, $(1,7)$max, $(2, -16)$min

4.3.3 Chain rule

1. $\dfrac{\mathrm{d}y}{\mathrm{d}x} = 2\sin x \cos x$
2. $\dfrac{\mathrm{d}y}{\mathrm{d}x} = 4e^{4x}\cos(e^{4x})$
3. $\dfrac{\mathrm{d}y}{\mathrm{d}x} = (14x + 2)e^{(7x^2 + 2x)}$
4. $\dfrac{\mathrm{d}y}{\mathrm{d}x} = 9(x - 1)^8$

4.3.4 Applied questions

1.

$$V = \frac{-3\mu_1\mu_2}{4\pi\varepsilon_0 r^4}$$

2.   •

a.
$$\frac{\mathrm{d}I}{\mathrm{d}\lambda} = -4I_0 \frac{\pi\alpha^2}{\varepsilon_r^2 \lambda^5 r^2} (\sin\phi)^2$$

b.
$$\frac{\mathrm{d}I}{\mathrm{d}\phi} = 2I_0 \frac{\pi\alpha^2}{\varepsilon_r^2 \lambda^4 r^2} (\sin\phi)(\cos\phi)$$

c.
$$\frac{\mathrm{d}I}{\mathrm{d}r} = -2I_0 \frac{\pi\alpha^2}{\varepsilon_r^2 \lambda^4 r^3} (\sin\phi)^2$$

3. $\dfrac{\mathrm{d}V}{\mathrm{d}t} = 0.8\pi r^2$, $\dfrac{\mathrm{d}SA}{\mathrm{d}t} = 1.6\pi r$

Chapter 5

Week 5

5.1 Preliminary infomation

A recap of standard differentials...

$f(x) \equiv y$	$f'(x) \equiv \dfrac{\mathrm{d}y}{\mathrm{d}x}$
A	0
Ax^n	nAx^{n-1}
$\dfrac{A}{x^n} \equiv Ax^{-n}$	$-nAx^{-n-1}$
e^{Ax}	Ae^{Ax}
$A \ln Bx$	$\dfrac{A}{x}$
$\sin Ax$	$A \cos Ax$
$\cos Ax$	$-A \sin Ax$
$\tan Ax$	$-A \sec^2 Ax$
$Au + Bv$	$A\dfrac{\mathrm{d}u}{\mathrm{d}x} + B\dfrac{\mathrm{d}v}{\mathrm{d}x}$

If differentiating a function of a function we use the 'Chain Rule':

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}y}{\mathrm{d}u} \times \frac{\mathrm{d}u}{\mathrm{d}x}$$

If differentiate a function times a function we use the 'Product Rule', if :

$$y = uv$$

...where u and v are different functions of x. The first derivative of this compound function may be found using the general differential form for products:

$$\mathrm{d}(uv) = v\mathrm{d}u + u\mathrm{d}v \tag{5.1}$$

5.2   Partial differentiation

Any good scientist knows that you should only change one variable at a time to understand the effect it has on a system. This is exactly what partial differentiation does, although it recognises that there may be more than one variable in the system...

Partial differentiation uses a different notation to standard differentiation to denote there is more than one variable. Subscritps are used to denote variables which are kept constant.

If y is a function of both x and z, then we can differentiate with respect to either variable, in this case we treat the other variable as a constant and differentiate as we ever have. The notation for differentiating y with respect to z as x is kept constant would be:

$$\left(\frac{\partial y}{\partial z}\right)_x$$

In some circumstances you may wish to differentiate a function first by one variable and then by another, the notation is this case is:

$$\left(\frac{\partial^2 y}{\partial x \partial z}\right)$$

this is implying that the partial derivative of y with respect to x was determined first and then the partial derivate of that first derivative was determined with respect to z. It should not matter in which order you perform these functions, they should both yield the same answer.

5.3   Questions

5.3.1   Product rule questions

Differentiate the following using the product rule:

1. $y = xe^{7x} + 7xe^x$
2. $y = 5x\cos(2x)$
3. $y = \frac{\sin x}{x^2}$
4. $y = \tan x$

5.3.2 More complex differentiation questions

Differentiate the following (you will need to decide if you need the product rule or the chain rule):

1. $y = x \ln x$
2. $y = \sin^7(5x) + \cos^5(7x)$
3. $y = x^2 e^{x^2}$
4. $y = e^{\sin x^2}$

5.3.3 Partial differentiation questions

For the following function determine:

$\left(\frac{\partial y}{\partial z}\right)_x$, $\left(\frac{\partial y}{\partial x}\right)_z$, $\left(\frac{\partial^2 y}{\partial z^2}\right)_x$, $\left(\frac{\partial^2 y}{\partial x^z}\right)_z$, $\left(\frac{\partial^2 y}{\partial x \partial z}\right)$ and $\left(\frac{\partial^2 y}{\partial z \partial x}\right)$

1. $y = x^6 z - 3x^2 z^3 + x^2 z + 6z^6 + 5$
2. $y = e^{3x} + ze^{2x} + x^2 e^{-z} - z^2$
3. $y = \frac{\sin(3z)}{x} - \frac{1}{e^{3x} z^2}$
4. $y = \sin(3z^2 + 2xz + x^2)$*

*this one is involved - it uses both the chain and the product rule!

5.4 Answers

5.4.1 Product rule questions

1. $\frac{\mathrm{d}y}{\mathrm{d}x} = e^{7x} + 7xe^{7x} + 7e^x + 7xe^x$
2. $\frac{\mathrm{d}y}{\mathrm{d}x} = 5\cos(2x) - 10x\sin(2x)$
3. $\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\cos x}{x^2} - \frac{2\sin x}{x^3}$
4. $\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{1}{\cos^2 x}$

5.4.2 More complex differentiation questions

1. $\frac{\mathrm{d}y}{\mathrm{d}x} = \ln x + 1$
2. $\frac{\mathrm{d}y}{\mathrm{d}x} = 35\cos(5x)\sin^6(5x) - 35\sin(7x)\cos^4(7x)$
3. $\frac{\mathrm{d}y}{\mathrm{d}x} = 2xe^{x^2} + 2x^3 e^{x^2}$
4. $y = 2x\cos x^2 e^{\sin x^2}$

5.4.3   Partial differentiation questions

1. $\left(\frac{\partial y}{\partial z}\right)_x = x^6 - 9x^2z^2 + x^2 + 36z^5$, $\left(\frac{\partial y}{\partial x}\right)_z = 6x^5z - 6xz^3 + 2xz$, $\left(\frac{\partial^2 y}{\partial z^2}\right)_x = -18X^2z + 180z^4$, $\left(\frac{\partial^2 y}{\partial x^z}\right)_z = 30x^4z - 6z^3$, $\left(\frac{\partial^2 y}{\partial x \partial z}\right) = 6x^5 - 18xz^2 + 2x$ and $\left(\frac{\partial^2 y}{\partial z \partial x}\right) = 6x^5 - 18xz^2 + 2x$

2. $\left(\frac{\partial y}{\partial z}\right)_x = e^{2x} - x^2e^{-z} - 2z$, $\left(\frac{\partial y}{\partial x}\right)_z = 3e^{3x} + 2e^{2x}z + 2xe^{-z}$, $\left(\frac{\partial^2 y}{\partial z^2}\right)_x = x^2e^{-z} - 2$, $\left(\frac{\partial^2 y}{\partial x^z}\right)_z = 9e^{3x} + 4e^{2x}z + 2e^{-z}$, $\left(\frac{\partial^2 y}{\partial x \partial z}\right) = 2e^{2x} - 2xe^{-z}$ and $\left(\frac{\partial^2 y}{\partial z \partial x}\right) = 2e^{2x} - 2xe^{-z}$

3. $\left(\frac{\partial y}{\partial z}\right)_x = \frac{\cos(3z)}{x} + \frac{2}{e^{3x}z^3}$, $\left(\frac{\partial y}{\partial x}\right)_z = -\frac{\sin(3z)}{x^2} + \frac{3}{e^{3x}z^2}$, $\left(\frac{\partial^2 y}{\partial z^2}\right)_x = -9\frac{\sin(3z)}{x} - \frac{6}{e^{3x}z^4}$, $\left(\frac{\partial^2 y}{\partial x^z}\right)_z = \frac{2\sin(3z)}{x^3} - \frac{9}{e^{3x}z^2}$, $\left(\frac{\partial^2 y}{\partial x \partial z}\right) = \frac{-3\cos(3z)}{x^2} - \frac{6}{e^{3x}z^3}$ and $\left(\frac{\partial^2 y}{\partial z \partial x}\right) = \frac{-3\cos(3z)}{x^2} - \frac{6}{e^{3x}z^3}$

4. $\left(\frac{\partial y}{\partial z}\right)_x = (6z + 2x)\cos(3z^2 + 2xz + x^2)$, $\left(\frac{\partial y}{\partial x}\right)_z = (2z + 2x)\cos(3z^2 + 2xz + x^2)$, $\left(\frac{\partial^2 y}{\partial z^2}\right)_x = 2\cos(3z^2 + 2xz + x^2) - (2z + 2x)^2\sin(3z^2 + 2xz + x^2)$, $\left(\frac{\partial^2 y}{\partial x^z}\right)_z = 6\cos(3z^2 + 2xz + x^2) - (6z + 2x)^2\sin(3z^2 + 2xz + x^2)$, $\left(\frac{\partial^2 y}{\partial x \partial z}\right) = 2\cos(3z^2 + 2xz + x^2) - (2z + 2x)(6z + 2x)\sin(3z^2 + 2xz + x^2)$ and $\left(\frac{\partial^2 y}{\partial z \partial x}\right) = 2\cos(3z^2 + 2xz + x^2) - (2z + 2x)(6z + 2x)\sin(3z^2 + 2xz + x^2)$
if you can do this one you can do them all!!!

Chapter 6

Week 6

6.1 Preliminary infomation

Standard anti derivatives (or integrals...)

$f'(x) \equiv y$	$f(x) \equiv \int y \, \mathrm{d}x$	Conditions
A	$x + C$	
Ax^n	$\dfrac{A}{n+1}x^{n+1} + C$	$x \neq -1$
$\dfrac{A}{x} \equiv Ax^{-1}$	$A\ln x + C$	
$\dfrac{A}{Bx+d}$	$\dfrac{A}{B}\ln(Bx+d) + C$	
e^{Ax}	$\frac{1}{A}e^{Ax} + C$	
A^x	$\frac{A^x}{\ln A} + C$	
$A\ln x$	$A\left(x\ln x - x\right) + C$	
$\sin Ax$	$-\frac{1}{A}\cos Ax + C$	
$\cos Ax$	$\frac{1}{A}\sin Ax + C$	
$\tan Ax$	$-\frac{1}{A}\ln(\cos Ax) + C \equiv \frac{1}{A}\ln(\sec Ax) + C$	$-\frac{\pi}{2} < x < \frac{\pi}{2}$
$\frac{A}{x^2+B^2}$	$\frac{A}{B}\tan^{-1}\left(\frac{x}{B}\right) + C$	$B > 0$
$Ax^2 e^{Bx}$	$A\left(\frac{x^2}{B} - \frac{2x}{B^2} + \frac{2}{B^3}\right)e^{Bx} + C$	
$v(x)\frac{\mathrm{d}u(x)}{\mathrm{d}x}$	$u(x)v(x) - \int u(x)\frac{\mathrm{d}v(x)}{\mathrm{d}x} + C$	Integration by Parts
$Au + Bv$	$A\dfrac{\mathrm{d}u}{\mathrm{d}x} + B\dfrac{\mathrm{d}v}{\mathrm{d}x}$	

6.2 Questions

6.2.1 Basic integration practice

Integrate the following with respect to the variable specified:

1. $f'(x) = \frac{a}{x}$; x
2. $f'(x) = x^{\frac{3}{2}} + \frac{x^{\frac{1}{2}}}{2} - 2x^{-\frac{1}{2}}$, x
3. $f'(b) = \sin(ab)$; b
4. $f'(T) = a + bT + \frac{c}{T}$; T
5. $f'(t) = k$; t
6. $f'([A]) = \frac{1}{[A]}$, [A]
7. $f'([A]) = \frac{1}{[A]^2}$, [A]
8. $f'(t) = -e^{-kt}$, t

6.2.2   Differential equations

Solve the following differential equations as far as possible:

1. $\frac{\mathrm{d}\ln a}{\mathrm{d}z} = bz^2$
2. $\frac{\mathrm{d}[A]}{\mathrm{d}t} = -k[A]^2$, when t= 0, $[A] = [A]_0$
3. $\frac{\mathrm{d}p}{\mathrm{d}T} = \frac{p\Delta_{\mathrm{vap}}H}{RT^2}$; when $T = T_1$, $p = p_1$ and when when $T = T_2$, $p = p_2$
4. $\frac{\mathrm{d}w}{\mathrm{d}V} = -\frac{nRT}{V}$, when $V = V_{\mathrm{i}}$, w = 0 and when $V = V_{\mathrm{f}}$, w = w

6.3   Answers

6.3.1   Basic integration practice

1. $f(x) = a\ln x + C$
2. $f(x) = \frac{2}{5}x^{\frac{5}{2}} + \frac{x^{\frac{3}{2}}}{3} + 4x^{\frac{1}{2}} + C$
3. $f(b) = -\frac{1}{a}\cos(ab) + C$
4. $f(T) = aT + \frac{bT^2}{2} + c\ln T + C$
5. $f(t) = kt + C$
6. $f([A]) = \ln[A] + C$
7. $f([A]) = -\frac{1}{[A]} + C$
8. $f(t) = \frac{e^{-kt}}{k}$

6.3.2   Differential equations

1. $\ln a = \frac{bz^3}{3} + D$
2. $\frac{1}{[A]} = \frac{1}{[A]_0} + kt$
3. $\ln\frac{p_1}{p_2} = \frac{\Delta_{\mathrm{vap}}H}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$
4. $w = -nRT\ln\frac{V_f}{V_i}$