AH Chemistry: Inorganic Chemistry

Section 1a: Electromagnetic Radiation & Atomic Spectra

JAB chem

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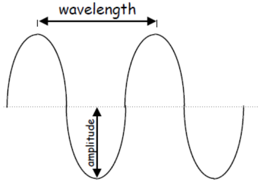
Electromagnetic radiation are waves that have both wavelength and frequency



Wavelength λ : (visible light wavelengths are usually given in nanometres)
the distance between wave crest to wave crest

Frequency f : (frequency is measured in Hertz)
the number of waves per second

Speed c :
All electromagnetic waves travel at 3×10^8 m s^{-1}

The equation c= f λ shows the relationship between wavelength and frequency.

$$c = f \times \lambda \qquad f = \frac{c}{\lambda} \qquad \lambda = \frac{c}{f}$$

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The radiation types of electromagnetic spectrum can be put in order of wavelength.

EM Radiation	Gamma rays	X rays	UV radiation	Visible light	Infra-Red radiation	Microwaves	Radio & TV waves
Wavelength	low ←						high
Frequency	high →						low
Energy	high →						low

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Electromagnetic radiation has a dual nature. It can be described as
- a wave with wavelength and frequency
- a particle

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Electromagnetic radiation can be absorbed or emitted by matter
- the radiation is behaving as a stream of particles called **photons**
- photons have quantised energy proportional to the frequency of the radiation
- higher the frequency the higher the energy (lower the wavelength the higher the energy)
- photons in high frequency radiation can transfer greater amounts of energy than photons in low frequency radiation.

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When a photon is absorbed, energy is gained by electrons being promoted to higher energy levels.
When a photon is emitted, energy is lost by an excited electron moving from higher energy level to a lower energy level

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The energy associated by a single photon is: $E = h \times f$ or $E = \frac{hc}{\lambda}$

As energy is often given in the unit kJ mol^{-1}

The energy associated by a one mole of photon is: $E = L \times h \times f$ or $E = \frac{Lhc}{\lambda}$

Symbol	*Quantity*	*Units*
E	Energy	kJ mol^{-1}
L	Avogadro's Constant	6.02×10^{23} mol^{-1}
h	Plank's Constant	6.63×10^{-34} J s
f	Frequency	Hz or s^{-1}
λ	Wavelength	m

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Light energy emitted by an atom produces a spectrum that is made up of a series of lines at discrete (quantised) energy levels.
- this provides direct evidence for the existence of these energy levels.
- each element in sample produces characteristic absorption & emission spectra.
- These spectra can be used to identify and quantify the element.

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In absorption spectroscopy, electromagnetic radiation is directed at an atomised sample.
- radiation is absorbed as electrons are promoted to higher energy levels.
- an absorption spectrum is produced by measuring how the intensity of absorbed light varies with wavelength.

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In emission spectroscopy, high temperature is used to excite the electrons within atoms.
- As the electrons drop to lower energy levels, photons are emitted.
- emission spectrum of a sample is produced by measuring the intensity of light emitted at different wavelengths.

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In atomic spectroscopy, the concentration of an element within a sample is related to the intensity of light emitted or absorbed.

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Section 1b: Atomic Orbitals and Electronic Configurations

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Discrete lines observed in atomic spectra can be explained if electrons, like photons, also display the properties of both particles and waves.

- electrons behave as standing (stationary) waves in an atom and these are waves that vibrate in time but do not move in space.
- different sizes and shapes of standing wave possible around the nucleus, known as orbitals.

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25 Orbitals can hold a maximum of two electrons.

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26 There are four different shapes of orbitals, identified as s, p, d and f

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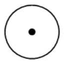
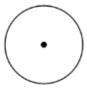
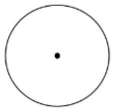
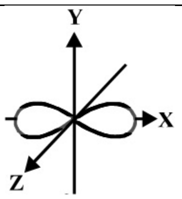
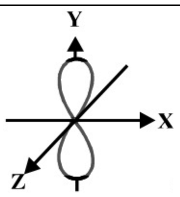
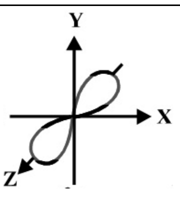
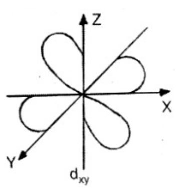
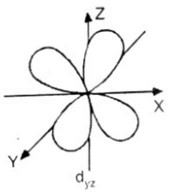
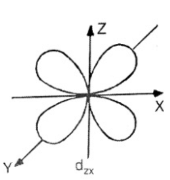
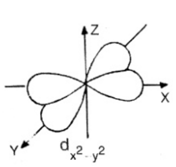
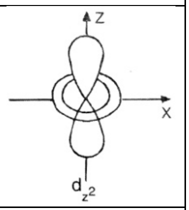
s orbital	 1s	 2s	 3s	s orbitals are circular and increase in size as value of n increases.	
p orbital	 2p$_x$	 2p$_y$	 2p$_z$	p orbitals are a figure of 8 shape which line along the one of axes	
d orbital					
f orbital	Not required to know f orbitals shapes for AH Chemistry.				

27 Electrons within atoms have fixed amounts of energy called quanta.

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28a The principal quantum number (n) is the shell number of an energy level.

- the higher the value of n the larger the size of the s-orbital.

Electron Shell	1st Shell	2nd Shell	3rd Shell	4th Shell	5th Shell
Principal Quantum number	n=1	n=2	n=3	n=4	n=5

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28b The angular momentum quantum numbers (l) describes the type of subshell within an electron shell.

- The values of l for each shell go from 0 up to n-1

Subshell Type	s	p	d	f
Angular Momentum Number	l=0	l=1	l=2	l=3

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28c The magnetic quantum numbers (m_l) describes the orientation of the orbitals within a subshell.

- values of each orbital go from –l through 0 up to +l

Subshell	Values of Magnetic Quantum Number (m_l)						
s (l=0)				0			
p (l=1)			-1	0	+1		
d (l=2)		-2	-1	0	+1	+2	
f (l=3)	-3	-2	-1	0	+1	+2	+3

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28d The spin magnetic quantum number (m_s) determines the spin direction of an electron and has values +½ or -½.

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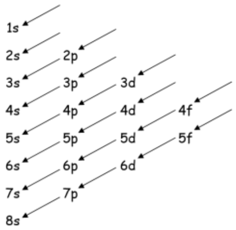
29a The aufbau principle states that electron orbitals fill up in order of increasing energy:

1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p, 8s



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29b Hund's rule states that electrons fill up orbitals singly first to maximise the number of parallel spins but filling each orbital with a second electron.

e.g. iron atoms have 26 electrons and has an electronic configuration of

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^6\ 4s^2$

1st five d-electrons fill up singly
6th d electrons doubles up.

↑↓	↑	↑	↑	↑

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29c	The Pauli exclusion principle states that • two electrons in the same atom cannot have the same four quantum numbers • no orbital can hold more than two electrons.		☹	😐	☺
30	In isolated atoms, orbitals within each subshell are degenerate (equal in energy)		☹	😐	☺
31	I can represent the relative energies corresponding to each orbital diagrammatically for the first four shells of a multi-electron atom using orbital box notation.		☹	😐	☺

32 ☹ 😐 ☺

Electron configuration of the first 36 elements using orbital box or spectroscopic notation can be written.

Element	Electronic Configuration							
	Spectroscopic Notation	Orbital Box Notation						
		1s	2s	2p	3s	3p	3d	4s
Scandium	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^1\ 4s^2$	↑↓	↑↓	↑↓ ↑↓ ↑↓	↑↓	↑↓ ↑↓ ↑↓	↑ ☐ ☐ ☐ ☐	↑↓
Vanadium	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^3\ 4s^2$	↑↓	↑↓	↑↓ ↑↓ ↑↓	↑↓	↑↓ ↑↓ ↑↓	↑ ↑ ↑ ☐ ☐	↑↓
Cobalt	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^7\ 4s^2$	↑↓	↑↓	↑↓ ↑↓ ↑↓	↑↓	↑↓ ↑↓ ↑↓	↑↓ ↑↓ ↑ ↑ ↑	↑↓

33 ☹ 😐 ☺

The periodic table is subdivided into four blocks (s, p, d and f) corresponding to the outer electronic configurations of the elements within these blocks.

s block	p block	d block	f block
Groups 1→2	Groups 3→0	Transition Metals	Actinides and Lanthanides.

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Variation in 1st, 2nd and subsequent ionisation energies with increasing atomic number for the first 36 elements is due to the relative stability of different subshell electronic configurations and this provides evidence for these electronic configurations. e.g.

Element	Electron Configuration	1st Ionisation Energy
Lithium	$1s^2\ 2s^1$	$\Delta H = +526\ kJ\ mol^{-1}$
Beryllium	$1s^2\ 2s^2$	$\Delta H = +905\ kJ\ mol^{-1}$
Boron	$1s^2\ 2s^2\ 2p^1$	$\Delta H = +807\ kJ\ mol^{-1}$
Carbon	$1s^2\ 2s^2\ 2p^2$	$\Delta H = +1090\ kJ\ mol^{-1}$

Removing an electron from Beryllium involves breaking a relatively stable $2s^2$ shell so requires more energy to remove an electron

1s	2s	2p
↑↓	↑↓	☐ ☐ ☐

Boron has $2p^1$ and removing an electron removes the entire 2p shell and leaves behind the more stable full $2p^2$

1s	2s	2p
↑↓	↑↓	↑ ☐ ☐

Element	Electron Configuration	1st Ionisation Energy
Carbon	$1s^2\ 2s^2\ 2p^2$	$\Delta H = +1090\ kJ\ mol^{-1}$
Nitrogen	$1s^2\ 2s^2\ 2p^3$	$\Delta H = +1410kJ\ mol^{-1}$
Oxygen	$1s^2\ 2s^2\ 2p^4$	$\Delta H = +1320\ kJ\ mol^{-1}$
Fluorine	$1s^2\ 2s^2\ 2p^5$	$\Delta H = +1690\ kJ\ mol^{-1}$

Nitrogen is harder to remove an electron from as it has a relatively stable half-filled 2p shell with parallel sins on the single electrons.

1s	2s	2p
↑↓	↑↓	↑ ↑ ↑

Oxygen is easier to remove an electron from as it creates a half-filled 2p shell.

1s	2s	2p
↑↓	↑↓	↑↓ ↑ ↑

Anomalies in ionisation energy trends are explained by considering electronic configurations.

- there is a special stability associated with half-filled and full subshells
- the more stable the electronic configuration, the higher the ionisation energy.

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VSEPR (valence shell electron pair repulsion) theory is used to predict the shapes of molecules and polyatomic ions.

The number of electron pairs surrounding a central atom is calculated by:

$$\text{Electron pairs} = \frac{\text{Number of electrons around central atom} + \text{number of bonds} - \text{charge}}{2}$$

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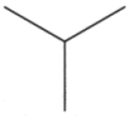
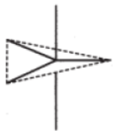
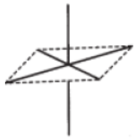
Electron pairs are negatively charged and repel each other

- electron pairs are arranged to minimise repulsion and maximise separation.
- both lone pairs and bonding pairs take part in deciding the shape of the electron pairs around the central atom.

2 electron pairs	3 electron pairs	4 electron pairs	5 electron pairs	6 electron pairs
F — Be — F				
Linear	Trigonal Planar	Tetrahedral	Trigonal Pyramidal	Octahedral

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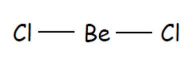
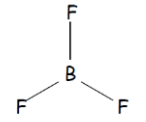
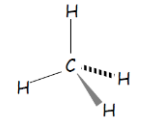
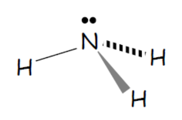
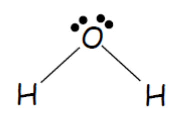
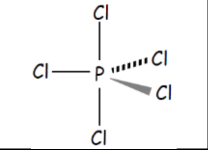
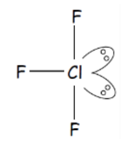
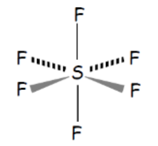
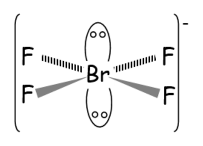
The shapes of molecules and polyatomic ions are determined by the shapes adopted by the atoms present based on the arrangement of electron pairs.

2 electron pairs	3 electron pairs	4 electron pairs	4 electron pairs	4 electron pairs
2 bonding + 0 lone pairs	3 bonding + 0 lone pairs	4 bonding + 0 lone pairs	3 bonding + 1 lone pairs	2 bonding + 2 lone pairs
				
Linear	Trigonal Planar	Tetrahedral	Trigonal Pyramidal	Angular

5 electron pairs	5 electron pairs	6 electron pairs	6 electron pairs
5 bonding + 0 lone pairs	3 bonding + 2 lone pairs	6 bonding + 0 lone pairs	4 bonding + 2 lone pairs
			
Trigonal Bipyramidal	T-Shaped	Octahedral	Square Planar

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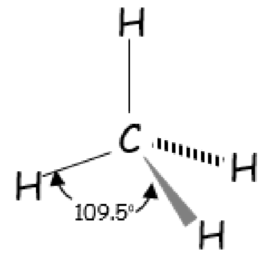
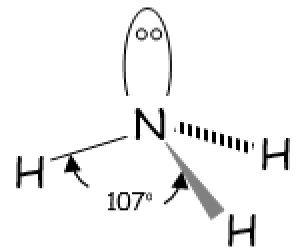
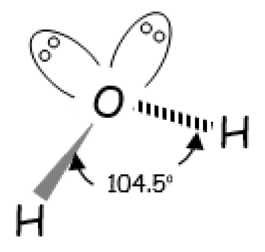
Electron pair repulsions decrease in strength in the order:
non-bonding pair/non-bonding pair > non-bonding pair/bonding pair > bonding pair/bonding pair

		
4 Bonding Pairs + 0 lone pairs	3 Bonding Pairs + 1 lone pairs	2 Bonding Pairs + 2 lone pairs
Angle between bonds = 109.5°	Angle between bonds = 107°	Angle between bonds = 104.5°

- Bond angle in NH_3 is narrower than in CH_4 as lone pair pushes bonding pairs closer together due to the increased repulsion of a lone pair compared to a bonding pair.
- Bond angle in H_2O is even narrower due top two lone pairs pushing them closer together

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Section 1c: Transition Metals

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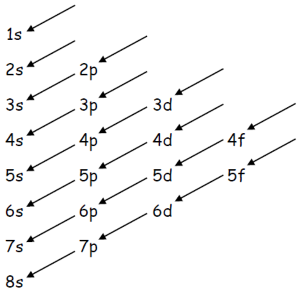
44 Metals with an incomplete d subshell in at least one of their ions are called d-block transition metals ☹ 😐 ☺

45 The aufbau principle states that orbitals of the lowest energy fill up first with electrons



Exceptions to aufbau rule include:

Element	Electronic Configuration according to aufbau principle	Actual Electronic configuration	Reason
Chromium	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^4\ 4s^2$	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5\ 4s^1$	Half-filled $3d^5$ preferred to full $4s^2$
Copper	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^9\ 4s^2$	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^1$	Full $3d^{10}$ preferred to full $4s^2$

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46 Electrons are lost from the outer electrons shell first, regardless of the order they fill up in according to the aufbau principle.

- In transition metals, 4s electrons are removed before 3d electrons when metal ions are formed.

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47 48 An element is in a particular oxidation state when it has a specific oxidation number.

- oxidation number in a free or uncombined element in zero
- for single atoms ions, the oxidation number is the same as the charge on the ion
- hydrogen usually has a oxidation number of +1 (except in hydrides)
- oxygen usually has an oxidation number of -2 (except in peroxides)
- The algebraic sum of all the oxidation numbers in a molecule must be zero
  e.g. In SO_3, three O atoms give 3x oxidation state of -2 and combine to equal -6
  therefore the sulphur must have the oxidation state of +6.
- The algebraic sum of all the oxidation numbers in a polyatomic ion must be equal to the charge on the ion
  e.g. In SO_4^{2-}, four O atoms give 4x oxidation state of -2 and combine to equal -8
  therefore the sulphur must have the oxidation state of +6 to allow the overall charge to equal -2.

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49 50 Transition metals can have different oxidation states in its compounds.

- compounds of the same transition metal in different oxidation states may have different colours e.g.

Ion	VO_3^-	VO^{2+}	V^{3+}	V^{2+}
Oxidation Sate of Vanadium	+5	+4	+3	+2
Colour	Yellow	Blue	Green	Violet

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51 52 Oxidation occurs when the oxidation number of a species increases
Reduction occurs when the oxidation number of a species decreases ☹ 😐 ☺

53 Compounds containing metals in high oxidation states are often oxidising agents.

- Oxidising agents are reduced themselves which reduces the oxidation number

Compounds with metals in low oxidation states are often reducing agents.

- Reducing agents are oxidised themselves which increases the oxidation number

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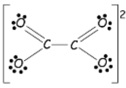
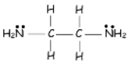
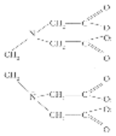
54 55 A ligand is defined as a molecule or ion electron donor which bonds to the metal ion by the donation of one or more electron pairs to unfilled metal ion orbitals.

<table>
<tr><td>Type of Ligand</td><td>Monodentate</td><td colspan="2">Bidentate</td><td>Hexadentate</td></tr>
<tr><td>Example</td><td><table><tr><td>Neutral Ligands</td><td>Charged Ligands</td></tr><tr><td>Water OH_2</td><td>Chloride Cl^-</td></tr><tr><td>Ammonia NH_3</td><td>Cyanide CN^-</td></tr><tr><td>Carbon Monoxide CO</td><td>Nitrite NO_2^-</td></tr><tr><td></td><td>Hydroxide OH^-</td></tr></table></td><td>Oxalic acid $O_4C_2^{2-}$
</td><td>1,2-diaminoethane $N_2C_2H_8$
</td><td>E.D.T.A.
</td></tr>
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57 The total number of bonds of the ligand(s) to the central transition metal ion is called the co-ordination number

- EDTA has a co-ordination number of 6
- hexaaquacopper(II) $[Cu(OH_2)_6]^{2+}$ has a co-ordination number of 6 as the central Cu^{2+} ion is surrounded by 6 water molecules
- tetrachloridocuprate(II) $[CuCl_4]^{2-}$ has a co-ordination number of 4 as the central Cu^{2+} ion is surrounded by 4 negative chloride ions

☹ 😐 ☺

56
58

Naming of Complexes from Formula

- Ligands listed alphabetically followed by the name of the central metal ion
- Naming of ligands follow the following rules

Neutral Ligand	Naming
Water	aqua
Ammonia	ammine
Carbon monoxide	carbonyl

Charged Ligands	Naming
-ide ending ligand e.g. chlor**ide**	chlor**ido**
-ate ending ligand e.g. oxal**ate**	oxal**ato**
-ite ending ligand e.g. nitr**ite**	nitr**ito**

- Mono, di, tri, tetra, penta, prefixes are used for multiple ligands of the same type
- If complex ion is overall a negative ion, the suffix *–ate* is added to the metal
  - nickel becomes nickelate(II)
  - iron becomes ferrate(III) [not ironate]
  - copper becomes cuprate(II) [not copperate]
- If complex ion is overall a positive ion, the metal does not have the suffix *–ate*
- The oxidation state of the metal is written after the metal (roman numerals in brackets)

e.g. $[Co[NH_3)_6]^{2+}$ is hexaamminecobalt(II)
$[Fe(O_4C_2)_3\ )_6]^{3-}$ is trioxalatoferrate(III)

Writing Formula from Names of Complexes.

- formula of complex ions are written in square brackets
- metal symbol comes first
- ligands are listed alphabetically irrespective of being charged or neutral
- atom in ligand which donates pair of electrons written first e.g. OH_2 or $O_4C_2^{2-}$
- overall charge on complex ion written after square brackets

e.g. tetrachloridocuprate(II) is written as $[CuCl_4]^{2-}$
hexaaquacopper(II) is written as $[Cu(H_2O)_6]^{2+}$

☹ 😐 ☺

59
60
61

In a complex of a transition metal, the d orbitals are no longer degenerate (equal in energy)

- splitting of d orbitals to higher and lower energies occurs when the electrons present in approaching ligands cause the electrons in the orbitals lying along the axes to be repelled.
- weak field and strong field ligands affect energy differences between subsets of d orbitals.

☹ 😐 ☺

62

Ligands can be placed in a spectrochemical series based on their ability to split d orbitals.

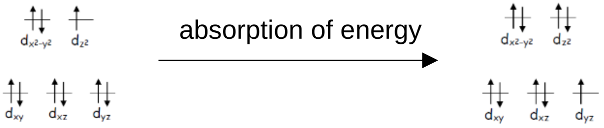
$$I^- < Br^- < Cl^- < F^- < H_2O < NH_3 < CN^-$$

☹ 😐 ☺

63
64
65

The colour of transition metal complexes can be explained in terms of d-d transitions.

- $dx^2–y^2$ and dz^2 orbitals are raised to a higher energy level due to electrostatic repulsion from the ligands in the complex
- transition metals can absorb light because photons (at a particular wavelength) excite electrons in the lower d-orbitals (ground state) up to a higher energy d-orbital (excited state)



- light of one colour is absorbed, then the complementary colour will be observed.
- electrons transition to higher energy levels when energy corresponding to the ultraviolet or visible regions of the electromagnetic spectrum is absorbed.

☹ 😐 ☺

66
67
68

Transition metals can act as catalysts as they can form a variable number of bonds due to the availability of unoccupied and half-filled d-orbitals

- allows the easier formation of intermediate complexes
- provides reaction pathways of lower energy to proceed
- variability of oxidation state of transition metals is important factor.
- transition metal reverts to original oxidation state once the reaction is complete

☹ 😐 ☺

69a

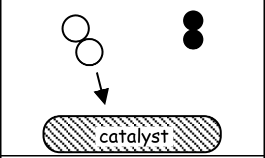
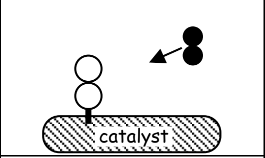
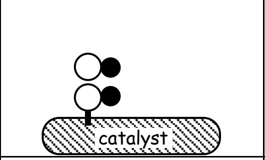
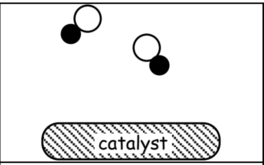
Homogeneous catalysts are in the <u>same</u> state as the reactants.

☹ 😐 ☺

69b
70

Heterogeneous catalysts are in the <u>different</u> state as the reactants.

- Heterogeneous catalysts work by the adsorption of reactant molecules

			
Reactant molecule collides with catalyst	Reactant molecule **adsorbs** to catalyst	Activated Complex forms	Product molecule(s) **desorbs** from catalyst

☹ 😐 ☺

AH Chemistry: Physical Chemistry

Section 2a: Chemical Equilibrium

JAB chem

			Traffic Light		
			red	amber	green
71 72	A chemical reaction is in equilibrium when the composition of the reactants and products remains constant indefinitely. - equilibrium constant (*K*) characterises the equilibrium composition of the reaction mixture		☹	😐	☺
73	For the general reaction: $aA + bB \rightleftharpoons cC + dD$ The equilibrium expression is: $K = \frac{[C]^c\,[D]^d}{[A]^a\,[B]^b}$ where: [A], [B], [C] & [D] are the equilibrium concentrations of A, B, C and D a, b, c & d are the stoichiometric coefficients in the balanced equation		☹	😐	☺
74 76	The value of equilibrium constant can be calculated: - the equilibrium constant has no units. e.g. 0.8mol of nitrogen and 1.5mol of hydrogen react by the Haber Process in a one litre container to give ammonia with an equilibrium concentration of 0.4mol. Equation: $N_2 + 3H_2 \rightleftharpoons 2NH_3$ Mole ratio: 1 mol, 3mol, 2mol 0.2mol, 0.6mol, 0.4mol (Reactants Left) (0.6mol leftover) (0.9mol leftover) As container has 1 litre volume, the number of moles is equal to concentration in mol l^{-1} $K = \frac{[NH_3]^2}{[N_2]\,[H_2]^3} = \frac{[0.4]^2}{[0.6] \times [0.9]^3} = 0.366$		☹	😐	☺
75	The value of the equilibrium constant K indicates the position of equilibrium. - A very high value of K (well above 1) indicated equilibrium far to the RIGHT - A very low value of K (well below 1) indicated equilibrium far to the LEFT		☹	😐	☺
77	Concentrations of pure solids and pure liquids at equilibrium are taken as constant and given a value of 1 in the equilibrium expression.		☹	😐	☺
78	The numerical value of the equilibrium constant depends on the reaction temperature and is independent of concentration and/or pressure.		☹	😐	☺
79	For endothermic reactions - a rise in temperature causes an increase in *K* - yield of the product is increased For exothermic reactions - a rise in temperature causes a decrease in *K* - yield of the product is decreased.		☹	😐	☺
80	The presence of a catalyst does not affect the value of the equilibrium constant.		☹	😐	☺
81	In water and aqueous solutions, water molecules form an equilibrium with hydronium and hydroxide ions. This ionisation of water can be represented by: $H_2O_{(l)} + H_2O_{(l)} \rightleftharpoons H_3O^+_{(aq)} + OH^-_{(aq)}$ water molecule, water molecule, hydronium ion, hydroxide ion		☹	😐	☺
82	Hydronium ion has the formula $H_3O^+_{(aq)}$ and is a hydrated proton and is often represented by the shorthand $H^+_{(aq)}$		☹	😐	☺
83	Water is described as amphoteric as it can act as an acid or a base.		☹	😐	☺
84 85	The dissociation constant K_w for the ionisation of water is known as the ionic product: $K_w = [H_3O^+]\,[OH^-]$ - value of K_w varies with temperature - K_w is approximately 1×10^{-14} at 25˚C.		☹	😐	☺
86	The relationship between pH and the hydronium H_3O^+ ion concentration is given by: $pH = -\log_{10}[H_3O^+]$ $[H_3O^+] = 10^{-pH}$		☹	😐	☺
87	In water and aqueous solutions with a pH value of 7, the concentrations of $H_3O^+_{(aq)}$ and $OH^-_{(aq)}$ are both equal to 10^{-7} mol l^{-1} at 25˚C.		☹	😐	☺
88	If the concentration of $H_3O^+_{(aq)}$ or $OH^-_{(aq)}$ is known, the concentration of the other ion can be calculated using the ionic product K_w (or by using pH + pOH = 14.) e.g. Calculate the $[OH^-]$ if $[H_3O^+] = 0.025$mol l^{-1} $[OH^-] = \frac{K_w}{[H_3O^+]} = \frac{1\times10^{-14}}{0.025} = 4\times10^{-13}$ mol l^{-1}		☹	😐	☺

89
90
91

The Brønsted-Lowry definition of acids and bases are:

Acid	Loses a proton (H^+) to form the conjugate base
Base	Gains a proton (H^+) to form the conjugate acid
Conjugate Acid	Formed when the base gains a proton (H^+)
Conjugate Base	Formed when the acid loses a proton (H^+)

For example:

$$\underset{\text{acid}}{CH_3COOH_{(aq)}} + \underset{\text{base}}{H_2O_{(l)}} \rightleftharpoons \underset{\text{conjugate base}}{CH_3COO^-_{(aq)}} + \underset{\text{conjugate acid}}{H_3O^+_{(aq)}}$$

☹ 😐 ☺

92

Strong acids fully dissociate into their ions

e.g. $HCl_{(g)} + H_2O_{(l)} \longrightarrow H_3O^+_{(aq)} + Cl^-_{(aq)}$

Weak acids partially dissociate into their ions

e.g. $CH_3COOH_{(l)} + H_2O_{(l)} \rightleftharpoons CH_3COO^-_{(aq)} + H_3O^+_{(aq)}$

☹ 😐 ☺

93
94

Examples of strong and weak acids & alkalis include:

Strong Acid	Weak Acid
hydrochloric acid	ethanoic acid
sulphuric Acid	carbonic acid
nitric Acid	sulphurous acid

Strong Base	Weak Base
Sodium hydroxide	Ammonia solution
Potassium hydroxide	
Lithium hydroxide	

☹ 😐 ☺

95

Carboxylic acids (and other weak acids) partially dissociate into ions, staying mainly as molecules.

Weak Acid	Equilibrium Equation
Ethanoic acid	$CH_3COOH_{(l)} + H_2O_{(l)} \rightleftharpoons CH_3COO^-_{(aq)} + H_3O^+_{(aq)}$
Sulphur Dioxide solution	$SO_{2(g)} + 2H_2O_{(l)} \rightleftharpoons 2H_3O^+_{(aq)} + SO_4^{2-}{}_{(aq)}$
Carbon Dioxide solution	$CO_{2(g)} + 2H_2O_{(l)} \rightleftharpoons 2H_3O^+_{(aq)} + CO_3^{2-}{}_{(aq)}$

☹ 😐 ☺

96

Ammonia, and amines, only partially dissociate into ions and mainly stays as molecules

Weak Base	Equilibrium Equation
Ammonia solution	$NH_{3(aq)} + H_2O_{(l)} \rightleftharpoons NH_4^+{}_{(aq)} + OH^-_{(aq)}$
1-aminomethane solution	$CH_3NH_{2(aq)} + H_2O_{(l)} \rightleftharpoons CH_3NH_3^+{}_{(aq)} + OH^-_{(aq)}$

☹ 😐 ☺

97

Equimolar solutions of weak and strong acids/bases have the following properties:

Property	Strong Acid	Weak Acid
pH Value	lower	Higher (Nearer pH=7)
Conductivity	Higher	Lower
Reaction Rate	Higher	Lower

Property	Strong Base	Weak Base
pH Value	higher	Lower (nearer pH=7)
Conductivity	Higher	Lower
Reaction Rate	Higher	Lower

☹ 😐 ☺

98

The acid dissociation constant or the equation $HA + H_2O \rightleftharpoons H_3O^+ + A^-$ is:

$$K_a = \frac{[H_3O^+]\,[A^-]}{[HA]} \qquad \therefore\ pK_a = -\log_{10} K_a$$

NB AS H_2O is both a reactant and the solvent, $[H_2O]$ is given the value = 1 and cancels out of equation.

☹ 😐 ☺

99

The approximate pH of a weak acid can be calculated using:

$$pH = \tfrac{1}{2}pK_a - \tfrac{1}{2}\log_{10}c$$

e.g. calculate the pH of 0.25mol l^{-1} solution of ethanoic acid ($pK_a = 4.76$)

$$\begin{aligned}
pH &= \tfrac{1}{2}pK_a &&- \tfrac{1}{2}\log_{10}c \\
pH &= \tfrac{1}{2}\times 4.76 &&- \tfrac{1}{2}\times \log_{10}(0.25) \\
pH &= 2.38 &&- \tfrac{1}{2}\times(-0.60) \\
pH &= 2.38 &&- (-0.30) \\
pH &= 2.68
\end{aligned}$$

☹ 😐 ☺

100

Acid Type	Base Type	pH of solution of Soluble Salt formed
Strong Acid	Strong Base	Neutral solution
Weak Acid	Strong Base	Alkaline solution
Strong Acid	Weak Base	Acidic Solution

☹ 😐 ☺

101

The names of salts are worked out from the individual acids and bases used:

Acid Used	Base Used	Name of Salt
hydrochloric acid	sodium hydroxide	sodium chloride
sulphuric acid	Potassium hydroxide	potassium sulphate
nitric acid	lithium hydroxide	lithium nitrate

Acid Used	Base Used	Name of Salt
ethanoic acid	magnesium hydroxide	magnesium ethanoate
sulphurous acid	calcium hydroxide	calcium sulphite
carbonic acid	ammonia solution	ammonium carbonate

☹ 😐 ☺

102

Salt solutions can have different concentrations of $H_3O^+_{(aq)}$ and $OH^-_{(aq)}$:

Sodium ethanoate solution has pH greater than 7	**Ammonium chloride solution has pH less than 7**
Sodium ethanoate solid fully dissociates into ions on dissolving.	Ammonium chloride solid fully dissociates into ions on dissolving.
Ethanoate ions collide with H_3O^+ ions to form molecules of ethanoic acid: $\underset{\text{ethanoate ion}}{CH_3COO^-_{(aq)}} + \underset{\text{hydronium ion}}{H_3O^+_{(aq)}} \rightleftharpoons \underset{\text{ethanoic acid molecule}}{CH_3COOH_{(aq)}} + \underset{\text{water}}{H_2O_{(l)}}$	Ammonium ions collide with hydroxide ions to form molecules of NH_3 $\underset{\text{ammonium ion}}{NH_4^+{}_{(aq)}} + \underset{\text{hydroxide ion}}{OH^-_{(aq)}} \rightleftharpoons \underset{\text{ammonia molecule}}{NH_{3(aq)}} + \underset{\text{water}}{H_2O_{(l)}}$
$H_3O^+_{(aq)}$ ions removed from solution as they join up with $CH_3COO^-_{(aq)}$ ions.	$OH^-_{(aq)}$ ions removed from solution as they join up with $NH_4^+{}_{(aq)}$ ions.
Equilibrium in water shifts to RIGHT to replace missing $H_3O^+_{(aq)}$ ions. $\underset{\text{water}}{H_2O_{(l)}} + \underset{\text{water}}{H_2O_{(l)}} \rightleftharpoons \underset{\text{hydronium ion}}{H_3O^+_{(aq)}} + \underset{\text{hydroxide ion}}{OH^-_{(aq)}}$	Equilibrium in water shifts to RIGHT to replace missing $OH^-_{(aq)}$ ions. $\underset{\text{water}}{H_2O_{(l)}} + \underset{\text{water}}{H_2O_{(l)}} \rightleftharpoons \underset{\text{hydronium ion}}{H_3O^+_{(aq)}} + \underset{\text{hydroxide ion}}{OH^-_{(aq)}}$
$[OH^-] > [H_3O^+]$ as $H_3O^+_{(aq)}$ ions are removed and $OH^-_{(aq)}$ build up	$[H_3O^+] > [OH^-]$ as $OH^-_{(aq)}$ ions are removed and $H_3O^+_{(aq)}$ build up

☹ 😐 ☺

103

Buffer solutions have a pH which remains approximately constant when small amounts of acid, base or water are added.

- Large amounts of acid or base will overpower the buffer solution.

☹ 😐 ☺

<table>
<tr><td>104</td><td>I can describe what an acidic and a basic buffer consists of.
<table>
<tr><th>Type</th><th>Description</th><th>Example</th></tr>
<tr><td>Acid Buffer</td><td>salt of weak acid dissolved in a weak acid</td><td>sodium ethanoate dissolved in ethanoic acid</td></tr>
<tr><td>Basic Buffer</td><td>salt of weak base dissolved in a weak base</td><td>ammonium chloride dissolved in ammonia solution</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>105</td><td>Acidic buffers and basic buffers work by the following mechanism:
<table>
<tr><th>Acid Buffer</th><th>Basic Buffer</th></tr>
<tr><td>e.g. sodium ethanoate dissolved in ethanoic acid solution.
$\overbrace{\underset{\text{ethanoic acid molecule}}{CH_3COOH_{(aq)}}}^{\text{large concentration from weak acid}} + \underset{\text{water}}{H_2O_{(l)}} \rightleftharpoons \overbrace{\underset{\text{ethanoate ion}}{CH_3COO^-_{(aq)}}}^{\text{large concentration from dissolved salt}} + \underset{\text{hydronium ion}}{H_3O^+_{(aq)}}$
<u>When acid is added to buffer</u>:
Equilibrium shifts to LEFT as added $H_3O^+_{(aq)}$ in added acid join up with ethanoate ions and form ethanoic acid molecules.
<u>When alkali is added to buffer</u>:
Equilibrium shifts to RIGHT as $H_3O^+_{(aq)}$ ions are neutralised by the alkali and ethanoic acid molecules dissociate into ions to replace $H_3O^+_{(aq)}$ ions.</td><td>e.g. ammonium chloride dissolved in ammonia solution.
$\overbrace{\underset{\text{ammonia molecule}}{NH_{3(aq)}}}^{\text{large concentration from weak acid}} + \underset{\text{water}}{H_2O_{(l)}} \rightleftharpoons \overbrace{\underset{\text{ammonium ion}}{NH_4^+{}_{(aq)}}}^{\text{large concentration from dissolved salt}} + \underset{\text{hydroxide ion}}{OH^-_{(aq)}}$
<u>When acid is added to buffer</u>:
Equilibrium shifts to RIGHT as $OH^-_{(aq)}$ ions are neutralised by the acid and ammonia NH_3 molecules dissociate into ions to replace $OH^-_{(aq)}$ ions.
<u>When alkali is added to buffer</u>:
Equilibrium shifts to LEFT as added $OH^-_{(aq)}$ in added alkali join up with ammonium NH_4^+ ions and form ammonia molecules.</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>106</td><td>The approximate pH of a buffer solution is calculated using:

$$pH = pK_a - \log_{10}\frac{[\text{acid}]}{[\text{salt}]}$$

e.g. Calculate the pH of a buffer where 3.74g of sodium ethanoate (CH_3COONa) is dissolved 0.20mol l^{-1} ethanoic acid and the final volume of the buffer is $100cm^3$.

gfm CH_3COONa = (2x12)+(3x1)+(2x16)+(1x23) = 24+3+32+23 = 82g mol^{-1}

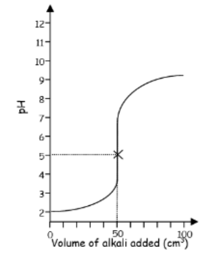
$$\textbf{n}\text{o. of mol} = \frac{\textbf{m}\text{ass}}{\textbf{gfm}} = \frac{3.74}{82} = 0.0456 \text{ mol}$$

$$\textbf{c}\text{oncentration} = \frac{\textbf{n}\text{o. of mol}}{\textbf{v}\text{olume}} = \frac{0.0456 \text{ mol}}{0.1 \text{ litres}} = 0.456 \text{ mol } l^{-1}$$

$$pH = pK_a - \log_{10}\frac{[\text{acid}]}{[\text{salt}]} = 4.76 - \log_{10}\frac{0.2}{0.456} = 4.76 - \log_{10}(0.439)$$
$$= 4.76 - (-0.358)$$
$$= 5.12$$</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>107</td><td>Indicators are weak acids in which the dissociation can be represented as:

$$HIn_{(aq)} + H_2O_{(l)} \rightleftharpoons H_3O^+_{(aq)} + In^-_{(aq)}$$</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>108</td><td>The dissociation constant K_{In} for an acid indicator is:

$$K_{In} = \frac{[H_3O^+][In^-]}{[HIn]}$$</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>109
110
111
112
113</td><td>The colour of an acid indicator is distinctly different from that of its conjugate base.

the colour of an indicator is determined by the ratio of [HIn] to $[In^-]$
the theoretical point at which colour changes is when $[H_3O^+] = K_{In}$
the colour change is assumed to be distinguished when [HIn] and $[In^-]$ differ by a factor of 10
the pH range over which a colour change occurs can be estimated by the expression: $pH = pK_a \pm 1$
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>114</td><td>Suitable indicators can be selected from pH data or titration curves.
<table>
<tr><td>Which of the following indicators should be used in the titration of aqueous potassium hydroxide solution with aqueous ethanoic acid
A. Phenolphthalein (pH range 8.3-10.0)
B. Bromothymol blue (pH range 6.0-7.6)
C. Methyl Red (pH range 4.2-6.3)
D. Methyl Orange (pH range 3.1-4.4)</td><td>Which indicator would be best in the following titration of ammonium hydroxide and sodium hydroxide?
<table>
<tr><td>
</td><td>A. Phenolphthalein (pH range 8.3-10.0)
B. Bromothymol blue (pH range 6.0-7.6)
C. Methyl Red (pH range 4.2-6.3)
D. Phenol Red (pH range 6.8-8.4)</td></tr>
</table></td></tr>
<tr><td>Answer:
Potassium hydroxide reacting with ethanoic acid will produce a salt solution with a pH in the alkaline region of the pH scale.
<i>Phenolphthalein</i> is the only listed indicator where the colour change pH range is entirely in the alkaline region of the pH scale.</td><td>Answer:
The titration curve clearly shows the neutralisation point to be around pH=5 so an indicator with a pH range of around 4.0-6.0 would be best used.
<i>Methyl Red</i> is the only list indicator which is close to this pH range.</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
</table>

AH Chemistry: Physical Chemistry

Section 2b: Reaction Feasibility

JAB chem

Traffic Light: red amber green

115 The standard enthalpy of formation, ΔH°_{f} is defined as the enthalpy change for the formation of one mole of a substance from its elements in their natural state.
e.g. Enthalpy of combustion of ethanol: $2C_{(s)} + 3H_{2(g)} + \frac{1}{2}O_{2(g)} \rightarrow C_2H_5OH_{(l)}$ ☹ 😐 ☺

116 Standard state of a substance is its most stable state at a pressure of 1 atmosphere and a specified temperature (usually 298K). ☹ 😐 ☺

117 I can calculate the standard enthalpy change of a reaction using:

$$\Delta H^{\circ} = \sum \Delta H^{\circ}_{f}\,(\text{products}) - \sum \Delta H^{\circ}_{f}\,(\text{reactants})$$

e.g. calculate ΔH° for the following reaction: $2ZnS_{(s)} + 3O_{2(g)} \rightarrow 2ZnO_{(s)} + 2SO_{2(g)}$

Substance	ΔH^{o}_{f} (kJ mol^{-1})
$2ZnS_{(s)}$	-206
$O_{2(g)}$	0
$ZnO_{(s)}$	-350
$2SO_{2(g)}$	-297

$$\begin{array}{lccc} \Delta H^{o} = & \Sigma\Delta H^{o}_{f}\,(\text{products}) & - & \Sigma\Delta H^{o}_{f}\,(\text{reactants}) \\ = & (2x\text{-}350) + (2x\text{-}297) & - & (2x\text{-}206)+(3x0) \\ = & (-700 - 594) & - & (-412 - 0) \\ = & -1294 & - & (-412) \\ = & -882\text{ kJ mol}^{-1} & & \end{array}$$

☹ 😐 ☺

118 119 120 121 Entropy (S) is a measure of the degree of disorder of a system
- the greater the degree of disorder, the greater the entropy
- solids have lower values of entropy than gases.
- entropy increases as temperature increases
- there is a large change in entropy at a substance's melting and boiling point
    - no change in temperature as state changes but large increase in entropy/disorder as solids turn into liquids or liquids turn into gas

☹ 😐 ☺

122 Second law of thermodynamics states that the total entropy of a reaction system and its surroundings always increases for a spontaneous process. ☹ 😐 ☺

123 124 When heat is released by a reaction system to the surroundings there is an increase in the entropy (disorder) of the surroundings.
- when heat is absorbed by a reaction system to the surroundings there is a decrease in the entropy (disorder) of the surroundings.

☹ 😐 ☺

125 Third law of thermodynamics states that the entropy of a perfect crystal at 0 K is zero. ☹ 😐 ☺

126 The standard entropy of a substance is the entropy content of one mole of a substance at 1atm pressure and 298K ☹ 😐 ☺

127 I can calculate the change in standard enthalpy of a reaction using:

$$\Delta S^{\circ} = \sum \Delta S^{\circ}(\text{products}) - \sum \Delta S^{\circ}(\text{reactants})$$

e.g. calculate ΔS° for the following reaction: $2ZnS_{(s)} + 3O_{2(g)} \rightarrow 2ZnO_{(s)} + 2SO_{2(g)}$

Substance	ΔS^{o} (J K^{-1} mol^{-1})
$2ZnS_{(s)}$	58
$O_{2(g)}$	205
$ZnO_{(s)}$	44
$2SO_{2(g)}$	248

$$\begin{array}{lccc} \Delta S^{o} = & \Sigma S^{o}(\text{products}) & - & \Sigma\Delta H^{o}_{f}\,(\text{reactants}) \\ = & (2x44) + (2x248) & - & (2x\text{-}206)+(3x0) \\ = & 88 + 496 & - & (-412 - 0) \\ = & 584 & - & (-412) \\ = & -147\text{ J K}^{-1}\text{ mol}^{-1} & & \end{array}$$

☹ 😐 ☺

128 I know that the change in free energy for a reaction is related to the enthalpy and entropy changes by:

$$\Delta G^{\circ} = \Delta H^{\circ} - T\Delta S^{\circ}$$

Free Energy (kJ mol^{-1})	=	Enthalpy Change (kJ mol^{-1})	–	Temperature x (K)	Entropy Change (kJ K^{-1} mol^{-1})

e.g. calculate ΔG° for the following reaction: $2ZnS_{(s)} + 3O_{2(g)} \rightarrow 2ZnO_{(s)} + 2SO_{2(g)}$ at 7000K

$$\begin{array}{lclcccc} \Delta G^{\circ} & = & \Delta H^{\circ} & - & T & x & \Delta S^{\circ} \\ \Delta G^{\circ} & = & -882 & - & 7000 & x & {}^{-147}/_{1000} \\ \Delta G^{\circ} & = & -882 & - & 5000 & x & -0.147 \\ \Delta G^{\circ} & = & -882 & - & & (-735) & \\ \Delta G^{\circ} & = & -147\text{ kJ mol}^{-1} & & & & \end{array}$$

Please note: entropy values of ΔS^{o} are usually given in J K^{-1} mol^{-1} so must be divided by 1000 to get them into kJ K^{-1} mol^{-1} when using this equation.

☹ 😐 ☺

129 When the change in free energy (ΔG°) between reactants and products is **negative**, a reaction may occur and the reaction is said to be **feasible**. ☹ 😐 ☺

130 A feasible reaction is one that tends towards the products rather than the reactants. This does not give any indication of the rate of the reaction. ☹ 😐 ☺

131 The standard free energy change for a reaction can be calculated using:

$$\Delta G^{\circ} = \sum \Delta G^{\circ}(\text{products}) - \sum \Delta G^{\circ}(\text{reactants})$$

☹ 😐 ☺

<table>
<tr><th></th><th></th><th></th><th></th><th></th><th></th></tr>
<tr><td>132
135</td><td>The feasibility of a chemical reaction under standard conditions can be predicted from the calculated value of the change in standard free energy (ΔG°).
<table>
<tr><td>When $\Delta G^o < 0$
Reaction is feasible</td><td>When $\Delta G^o = 0$
Reaction is just feasible
(reaction is in equilibrium)</td><td>When $\Delta G^{o`1234567} > 0$
Reaction is not feasible</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>133</td><td>I can estimate the temperatures at which a reaction may be feasible by considering the range of values of T for which $\Delta G^{\circ} < 0$.

e.g. calculate the temperature when the reaction becomes feasible:
$2ZnS_{(s)} + 3O_{2(g)} \rightarrow 2ZnO_{(s)} + 2SO_{2(g)}$
$\Delta G^o = \Delta H^o - T\Delta S^o = 0 \; \therefore \; T = \frac{\Delta H^o}{\Delta S^o} = \frac{-882 \times 1000 \text{ J mol}^{-1}}{-147 \text{ J K}^{-1} \text{ mol}^{-1}} = 6000\text{K}$</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>134</td><td>Any reaction is feasible if ΔG is negative, even under non-standard conditions</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>136</td><td>A reversible reaction will proceed spontaneously until the composition is reached where $\Delta G = 0$.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
</table>

AH Chemistry: Physical Chemistry

Section 2c: Kinetics

Traffic Light: red ☹ | amber 😐 | green ☺

137 Chemical reactions normally depend on the concentration of reactants ☹ 😐 ☺

138
139 The order of reaction with respect to each reactant can be determined by changing the concentration of each reactant individually. ☹ 😐 ☺

- The order of reaction relates each reacting species to the rate of reaction.

For the reaction: $A + B + C \longrightarrow D$

- Each reactant is varied one at a time and the reaction rate is measured:

Experiment	[A] (mol l^{-1})	[B] (mol l^{-1})	[C] (mol l^{-1})	Initial Rate of Reaction (mol l^{-1} s^{-1})
1	1.0	1.0	1.0	2.0
2	2.0	1.0	1.0	4.0
3	1.0	2.0	1.0	2.0
4	1.0	1.0	2.0	8.0

- Each reactant is compared to determine the effect of change of that reactant on the reaction rate

Experiments Compared	Change in Conditions	Effect of Change on Rate	Order of Reactant
1+2	[A] x2	rate x2	$[A]^1$
1+3	[B] x2	no change in rate	$[B]^0$
1+4	[C] x2	rate x4	$[C]^2$

- The order of the reactant can be assessing the effect of changing concentration on rate

140
141
142 The rate equation for a reaction can be written using the individual orders for each reactant. ☹ 😐 ☺

$$\text{Rate} = k \quad [A]^1 \quad \times \quad [B]^0 \quad \times \quad [C]^2$$

$$\text{Rate} = k \quad [A] \quad \times \quad 1 \quad \times \quad [C]^2$$

$$\text{Rate} = k \quad [A] \quad \times \quad [C]^2$$

143 The overall rate of a reaction can be determined from the rate equation. ☹ 😐 ☺

$$\text{Overall Order} = 1 + 0 + 2 = 3$$

144 The order of a reaction can only be determined form experimental data. ☹ 😐 ☺

145 Using the rate equation and data of initial rate in the results table, the value of the rate constant and units of the rate constant can be calculated. ☹ 😐 ☺

- reactants can be zero, first, second or third order

$$\text{Rate} = k \quad [A] \quad \times \quad [C]^2$$

$$2.0 \text{ mol } l^{-1} s^{-1} = k \quad [1.0\text{mol } l^{-1}] \quad \times \quad [1.0\text{mol } l^{-1}]^2$$

$$k = \frac{2.0 \text{ mol } l^{-1} s^{-1}}{1.0\text{mol } l^{-1} \times 1.0\text{mol}^2 \, l^{-2}}$$

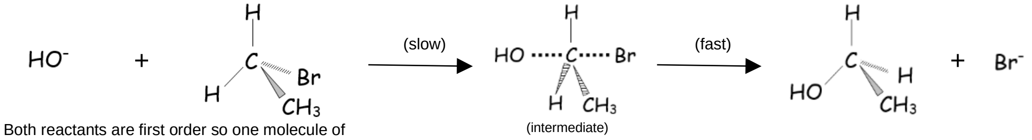
$$k = \frac{2.0 \text{ mol } l^{-1} s^{-1}}{1.0\text{mol}^3 \, l^{-3}}$$

$$k = 2.0 \; l^2 \text{ mol}^{-2} s^{-1}$$

146
147 Reactions usually occur by a series of steps called a reaction mechanism. The rate of the reaction is dependent on the slowest step called the rate determining step. ☹ 😐 ☺

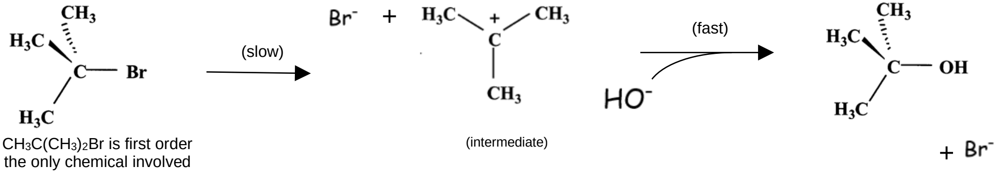
148 Reaction mechanisms can be worked out from experimentally determined rate equations ☹ 😐 ☺

For reaction: $CH_3CH_2Br + OH^- \rightarrow CH_3CH_2OH + Br^-$
Experiments show reactants have order $[OH^-]^1$ and $[CH_3CH_2Br]^1$



Both reactants are first order so one molecule of each takes part in the slow *rate determining step*

For the reaction: $CH_3C(CH_3)_2Br + OH^- \rightarrow CH_3C(CH_3)_2OH + Br^-$
Experiments show reactants have order $[OH^-]^0$ and $[CH_3C(CH_3)_2Br]^1$



Only $CH_3C(CH_3)_2Br$ is first order so is the only chemical involved in the slow rate determining step

AH Chemistry: Organic Chemistry

Section 3a: Molecular Orbitals

JAB chem

			Traffic Light		
			red	amber	green
149 150	I know that VSEPR cannot explain the bonding in all compounds and that molecular theory can provide an explanation for more complex molecules. I know that molecular orbits form when atomic orbitals combine and the number of molecular orbitals formed is equal to the number of atomic orbitals that combine.		☹	😐	☺
151 152	I know that the combination of two atomic orbitals results in the formation of a bonding molecular orbital and an antibonding orbital. I know that the bonding molecular orbital encompasses both nuclei.		☹	😐	☺
153 154	I know that the attraction of the positively charged nuclei and the negatively charged electrons in the bonding molecular orbital is the basis of bonding between atoms. I know that each molecular orbital can hold a maximum of two electrons.		☹	😐	☺
155 156 157	I know that in a non-polar covalent bond, the bonding molecular orbital is symmetrical about the midpoint between two atoms. I know that polar covalent bonds result from bonding molecular orbitals that are asymmetric about the midpoint between two atoms. I know that the atom with the greater value for electronegativity has the greater share of the bonding electrons.		☹	😐	☺
158	I know that ionic compounds are an extreme case of asymmetry, with the bonding molecular orbitals being almost entirely located around just one atom, resulting in the formation of ions.		☹	😐	☺
159	I can describe sigma (σ) molecular orbitals or sigma bonds.		☹	😐	☺
160	I can describe pi (π) molecular orbitals or pi bonds.		☹	😐	☺
161	I know that the electronic configuration of an isolated carbon atom cannot explain the number of bonds formed by carbon atoms in molecules and that the bonding and shape of molecules of carbon can be explained by hybridisation.		☹	😐	☺
162b 163	I can describe sp^3 hybridisation. I know that bonding in alkanes can be described in terms of sp^3 hybridisation.		☹	😐	☺
162a 164 165	I can describe sp^2 hybridisation. I know that bonding in alkenes can be described in terms of sp^2 hybridisation. I know that bonding in benzene and other aromatics can be described in terms of sp^2 hybridisation.		☹	😐	☺
166	I know that bonding in alkynes can be described in terms of sp hybridisation.		☹	😐	☺
167	I can describe the bonding in alkanes, alkenes, aromatics and alkynes in terms of sigma (σ) and pi bonds (π).		☹	😐	☺
168 169	I know that molecular orbital theory can be used to explain why organic molecules are colourless or coloured. I know that electrons fill bonding molecular orbitals, leaving higher energy antibonding orbitals unfilled.		☹	😐	☺
170	I know that the highest bonding molecular orbital containing electrons is called the highest occupied molecular orbital (HOMO) and the lowest antibonding molecular orbital is called the lowest unoccupied molecular orbital (LUMO).		☹	😐	☺
171 172	I know that absorption of electromagnetic energy can cause electrons to be promoted from HOMO to LUMO. I can explain why most organic molecules are colourless in terms of the energy difference between the HOMO and LUMO.		☹	😐	☺
173	I know that a chromophore is a group of atoms within a molecule that is responsible for absorption of light in the visible region of the spectrum.		☹	😐	☺
173 174 175	I know that a chromophore is a group of atoms within a molecule that is responsible for absorption of light in the visible region of the spectrum. I know that chromophores exist in molecules with a conjugated system and that a conjugated system is a system of adjacent unhybridised p orbitals that overlap side-on to form a molecular orbital across a number of carbon atoms where electrons are delocalised.		☹	😐	☺
176	I can explain the colours of compounds in terms of energy gap between the HOMO and LUMO, and the wavelength of light absorbed.		☹	😐	☺

AH Chemistry: Organic Chemistry

Section 3b: Synthesis

Traffic Light: red | amber | green

177
178

In organic reactions, bonds in the reactant molecules are broken and bonds in the product molecules are formed.

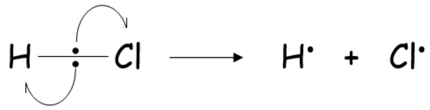
- the process of bond breaking is known as bond fission

☹ 😐 ☺

179
182a

Homolytic fission has a covalent bond splitting with one electrons going to either end of the bond to form free radicals (each with a unpaired electron)

- fish-hook style arrow represents the movement of one electron from the bond

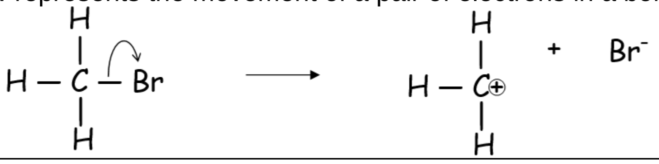


☹ 😐 ☺

180
182b

Heterolytic fission has a covalent bond splitting with both electrons going to one end of the bond to form a positive ion and negative ion.

- Full arrow represents the movement of a pair of electrons in a bond



☹ 😐 ☺

181
183

Reactions involving heterolytic fission tend to result in far fewer products than reactions involving homolytic fission

- heterolytic fission is better suited for organic synthesis as a result.
- in reactions involving heterolytic bond fission, attacking groups are classified as nucleophiles or electrophiles.

☹ 😐 ☺

184
185
186

Nucleophiles are attracted towards atoms bearing a partial (δ+) or full positive charge.

- nucleophiles that are capable of donating an electron pair can form a new covalent bond.

OH^-	CN^-	NH_3	O in H_2O	R^-
Negatively charged ions	Negatively charged ions	Molecules with lone pairs	Negatively polarised centres	carbanion

☹ 😐 ☺

187
188
189

Electrophiles are attracted towards atoms bearing a partial (δ-) or full negative charge.

- electrophiles that are capable of accepting an electron pair can form a new covalent bond.

H_3O^+	SO_3		H in H_2O	R^+
Positively charged ions			Positively polarised centres	carbocation

☹ 😐 ☺

190

There are different chemical reaction types shown in the following a chemical equations:

a) **substitution**: reaction with one atom/group replacing another atom/group

$$CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$$

b) **addition**: molecule adding across a C=C double bond or C≡C triple bond

$$C_2H_4 + Br_2 \longrightarrow C_2H_4Br_2$$

c) **elimination**: molecule removed leaving behind a C=C double bond

$$C_2H_5OH \longrightarrow C_2H_4 + H_2O$$

d) **condensation**: 2 molecules join together and a small molecule removed at join

$$\underset{\text{methanol}}{CH_3OH} + \underset{\text{ethanoic acid}}{CH_3COOH} \longrightarrow \underset{\text{methyl ethanoate}}{CH_3OCOCH_3} + \underset{\text{water}}{H_2O}$$

e) **hydrolysis**: molecules splits into 2 molecules with small molecule added at join

$$\underset{\text{methyl ethanoate}}{CH_3OCOCH_3} + \underset{\text{water}}{H_2O} \longrightarrow \underset{\text{methanol}}{CH_3OH} + \underset{\text{ethanoic acid}}{CH_3COOH}$$

f) **oxidation**: increase in oxygen : hydrogen ratio with a loss of electrons

$$\underset{\text{methanol}}{CH_3OH} + \tfrac{1}{2}O_2 \longrightarrow \underset{\text{methanoic acid}}{HCOOH} + H_2O$$

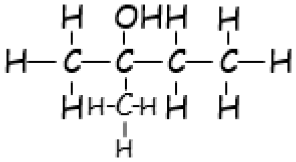
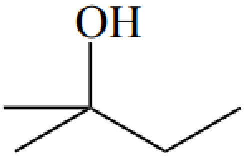
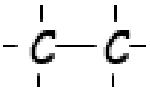
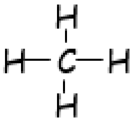
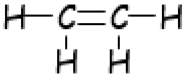
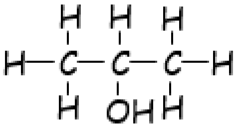
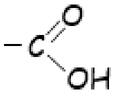
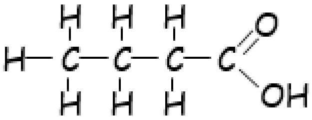
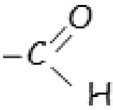
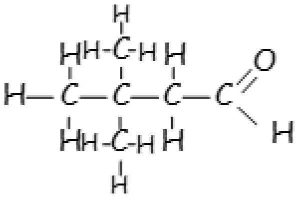
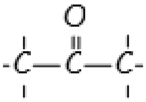
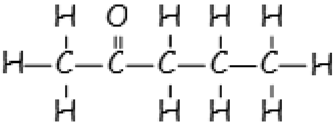
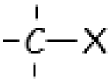
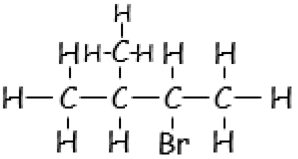
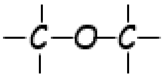
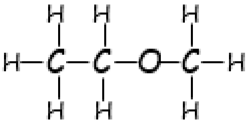
g) **reduction**: decrease in oxygen : hydrogen ratio with a gain of electrons

$$\underset{\text{propanone}}{CH_3COCH_3} + H_2O \longrightarrow \underset{\text{propan-2-ol}}{CH_3CH(OH)CH_3} + \tfrac{1}{2}O_2$$

h) **neutralisation**: acid and base reaction to form water and a salt

$$H_2SO_4 + Na_2O \longrightarrow Na_2SO_4 + H_2O$$

☹ 😐 ☺

<table>
<tr>
<td>191</td>
<td>Synthetic routes from given reactant to final product can be devised with up to 3 steps:
2-bromobutane → butan-2-ol → butanoic acid → methylbutanoate
nucleophilic substitution oxidation condensation</td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
<tr>
<td>192
193</td>
<td>Skeletal formulae can be used in addition to structure formula and molecular formula.
<table>
<tr><th>Structural Formula</th><th>Skeletal Formula</th><th>Molecular Formula</th></tr>
<tr><td rowspan="3"></td><td rowspan="3"></td><td>$C_5H_{12}O$</td></tr>
<tr><td>Shortened Structural Formula</td></tr>
<tr><td>$CH_3C(CH_3)(OH)CH_2CH_3$</td></tr>
</table>
</td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
<tr>
<td>194
196</td>
<td>The following homologous series can be named and drawn for examples up to 8 carbons:
<table>
<tr><th colspan="2">Homologous Series</th><th>Functional Group</th><th>General Formula</th><th>Example</th></tr>
<tr><td>a)</td><td>Alkanes</td><td>
(C-C single bonds)</td><td>C_nH_{2n+2}</td><td>
methane CH_4</td></tr>
<tr><td>b)</td><td>Alkenes</td><td>
C=C double bonds</td><td>C_nH_{2n}</td><td>
ethene C_2H_4</td></tr>
<tr><td>c)</td><td>Alcohols</td><td>
Hydroxyl group</td><td>$C_nH_{2n+1}OH$</td><td>
propan-2-ol C_3H_7OH</td></tr>
<tr><td>d)</td><td>Carboxylic Acids</td><td>
Carboxyl Group</td><td>$C_nH_{2n+1}COOH$</td><td>
butanoic acid C_3H_7COOH</td></tr>
<tr><td>e)</td><td>Aldehydes</td><td>
Aldehyde Group</td><td>$C_nH_{2n}O$</td><td>
3,3-dimethylbutanal $C_6H_{12}O$</td></tr>
<tr><td>f)</td><td>Ketones</td><td>
Ketone Group</td><td>$C_nH_{2n}O$</td><td>
pentan-2-one $C_5H_{10}O$</td></tr>
<tr><td>g)</td><td>Haloalkanes</td><td>
Halogen Group
(where X is F, Cl, Br or I)</td><td>$C_nH_{2n+1}X$</td><td>
2-bromo-3-methylbutane $C_5H_{11}Br$</td></tr>
<tr><td>h)</td><td>Ethers</td><td>
Ether Group</td><td>$C_nH_{2n+2}O$</td><td>
Methoxyethane</td></tr>
</table>

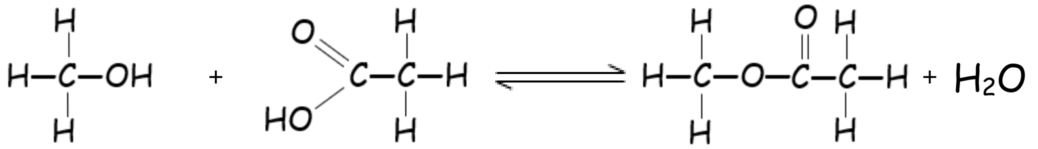
give systematic naming of straight or branched chain structures of the above homologous series with functional groups numbered where appropriate
give drawings and write molecular formulae of named straight or branched chain structures.

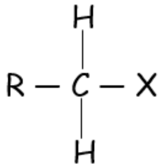
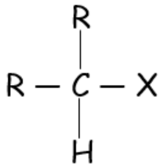
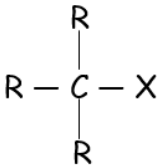
</td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
</table>

<table>
<tr>
<td>195
197</td>
<td>Straight chain esters can be systematically named from the names of their parent alcohol and carboxylic acid or the structural formula of the alcohol and carboxylic acid

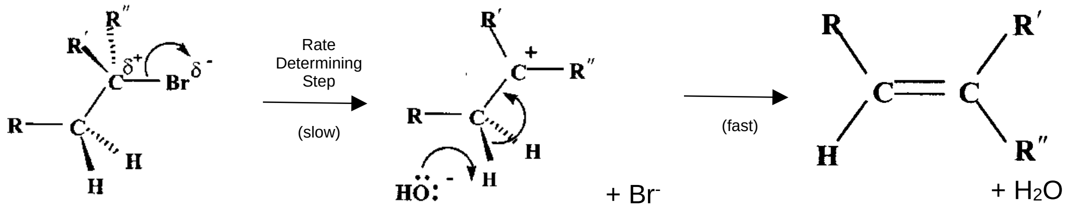
- Parent alcohol name comes first in ester name e.g. ethanol becomes *ethyl*
- Parent Carboxylic Acid name comes second in ester name e.g. propanoic acid becomes *propanoate*

Alcohol + Carboxylic Acid ⇌ Ester + Water

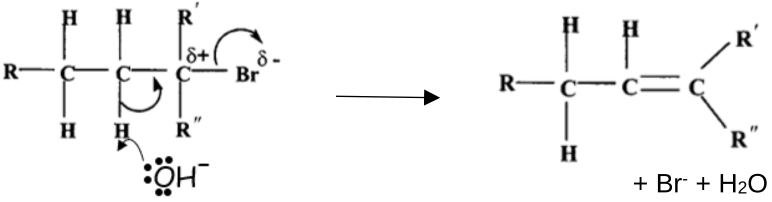


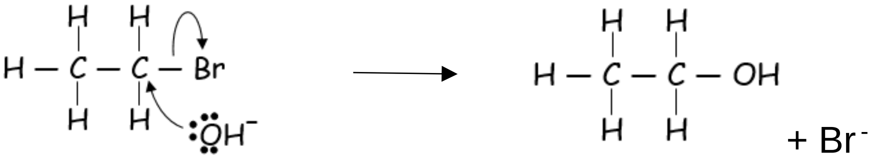
methanol + ethanoic acid ⇌ methyl ethanoate + water
CH_3OH CH_3COOH CH_3OCOCH_3 H_2O</td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
<tr>
<td>198
199</td>
<td>Haloalkanes (alkyl halides) are substituted alkanes in which one or more of the hydrogen atoms is replaced with a halogen atom.
<table>
<tr><th>Primary Haloalkanes</th><th>Secondary Haloalkanes</th><th>Tertiary Haloalkanes</th></tr>
<tr><td></td><td></td><td></td></tr>
<tr><td>1 alkyl group attached to the C atom with the halogen attached</td><td>2 alkyl group attached to the C atom with the halogen attached</td><td>3 alkyl group attached to the C atom with the halogen attached</td></tr>
</table></td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
<tr>
<td>200
222</td>
<td>monohaloalkanes can take part in elimination reactions to form alkenes using a strong base, such as potassium or sodium hydroxide dissolved in ethanol.

<u>E1 Mechanism</u>: 1 molecule involved in the rate determining state



<u>E2 Mechanism</u>: 2 molecules involved in the rate determining state

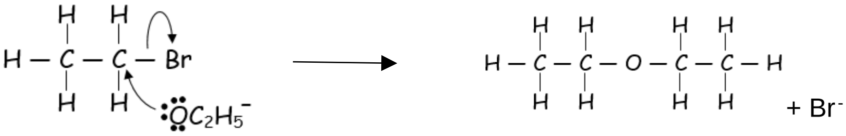

</td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
<tr>
<td>201a</td>
<td>Monohaloalkanes reacts with aqueous alkalis to form alcohols by nucleophilic substitution

</td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
<tr>
<td>201b
211</td>
<td>Monohaloalkanes react with alcoholic alkoxides to form ethers by nucleophilic substitution.

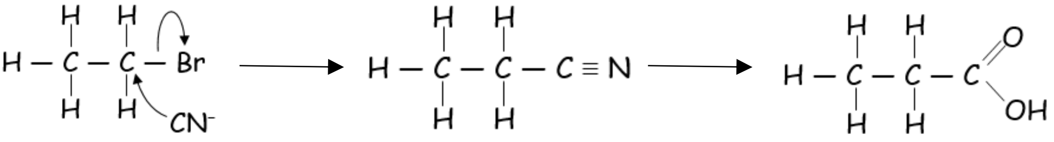
- Alkoxides made by reaction of Group 1 metal with alcohol

$Na(s) + C_2H_5OH(l) \longrightarrow H_2(g) + C_2H_5O^-Na^+$
ethanol sodium ethoxide

- Alkoxide ions then react with δ+ on Carbon of carbon–halogen bond

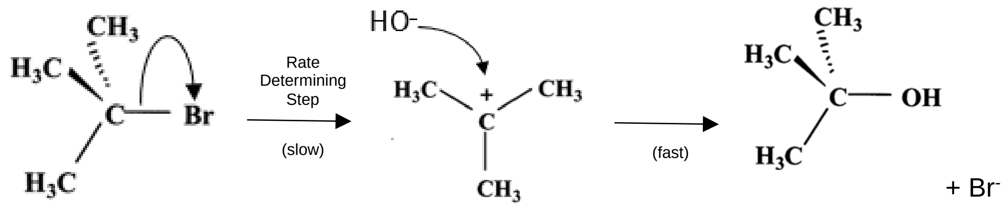
</td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
<tr>
<td>201c</td>
<td>Monohaloalkanes react with ethanolic cyanide to form nitriles by nucleophilic substitution

- chain length increased by one carbon atom
- can be hydrolysed to carboxylic acids

</td>
<td></td>
<td>☹</td>
<td>😐</td>
<td>☺</td>
</tr>
</table>

<table>
<tr><td>202
206</td><td>I know that a monohaloalkane can take part in nucleophilic substitution reactions by one of two different mechanisms.

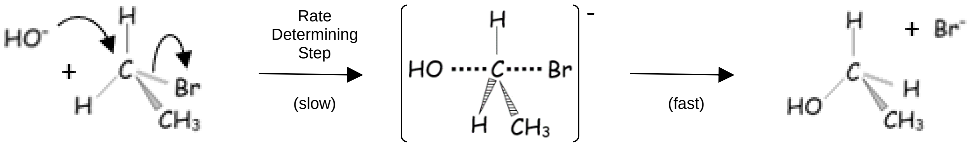
Tertiary haloalkanes tend to react via S_N1 reactions due to steric hindrance of the side groups in the tertiary haloalkane blocking the attack of the nucleophile for the $\delta+$ on the carbon atom in the carbon to halogen bond. Groups off this carbon provide inductive stabilisation of the carbocation intermediate.
Primary and Secondary haloalkanes tend to react via S_N2 reactions
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>203
205a</td><td>The mechanism of S_N1 nucleophilic substitution is:



curly arrows show movement of pair of electrons

carbocation intermediate

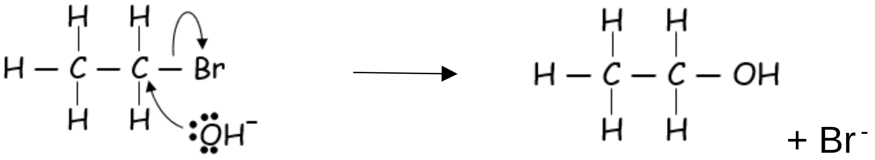
products</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>204
205b</td><td>The mechanism of S_N2 nucleophilic reactions is:

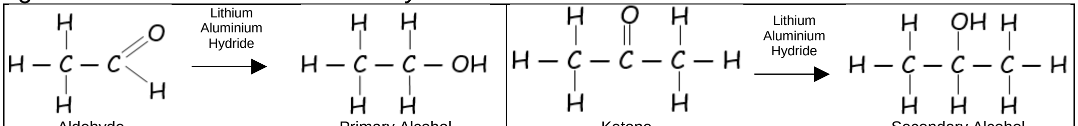


curly arrows show movement of pair of electrons

transition state

products</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>207</td><td>Alcohols are substituted alkanes in which one or more of the hydrogen atoms is replaced with a hydroxyl functional group, –OH group.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>208a</td><td>Alcohols can be prepared from haloalkanes by nucleophilic substitution


</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>208c</td><td>Alcohols can be prepared from aldehydes and ketones by reduction using a reducing agent such as lithium aluminium hydride



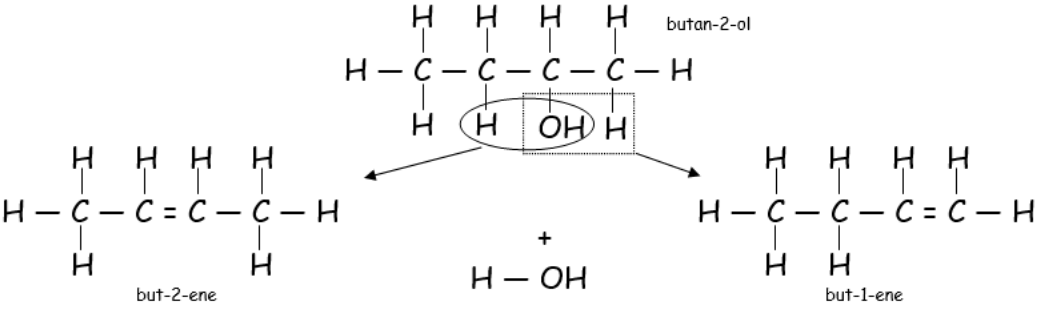
Aldehyde
ethanal

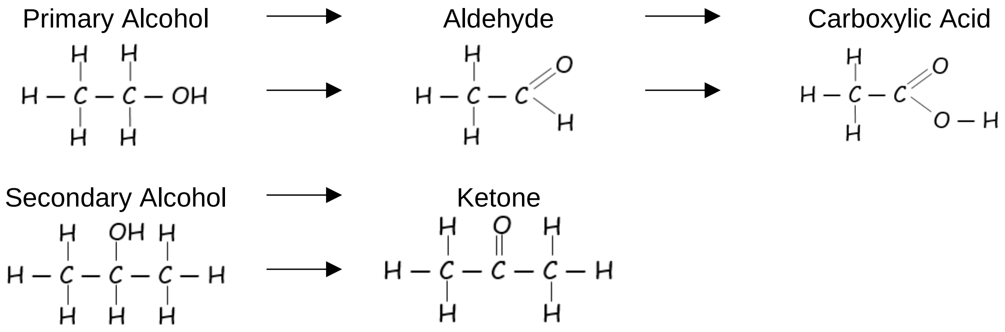
Primary Alcohol
ethanol

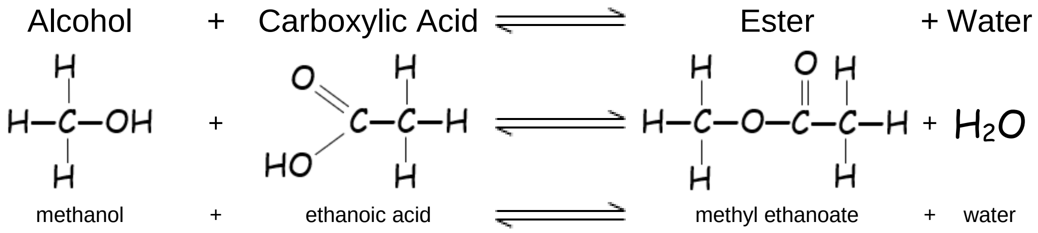
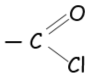
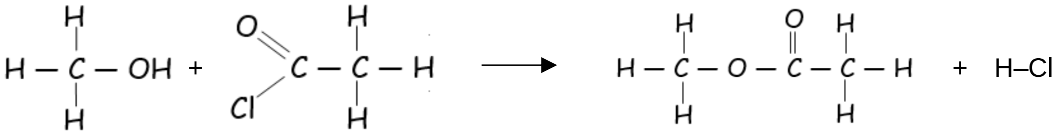
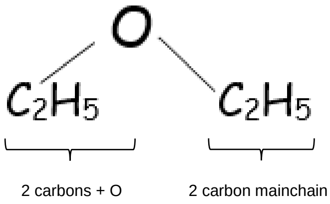
Ketone
propanone

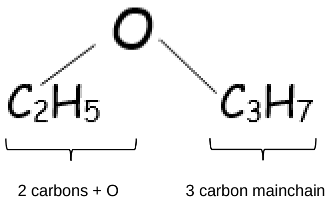
Secondary Alcohol
propan-2-ol</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>209</td><td>Alcohols can be dehydrated to form alkenes using one of:

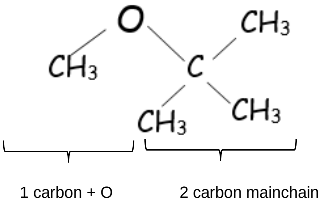
<table><tr><td>aluminium oxide</td><td>concentrated sulphuric acid</td><td>concentrated phosphoric acid</td></tr></table>

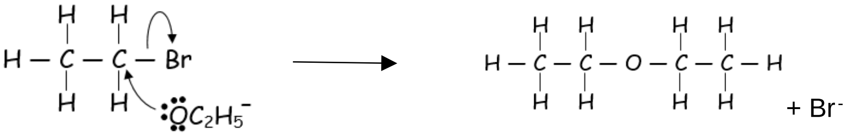

</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
</table>

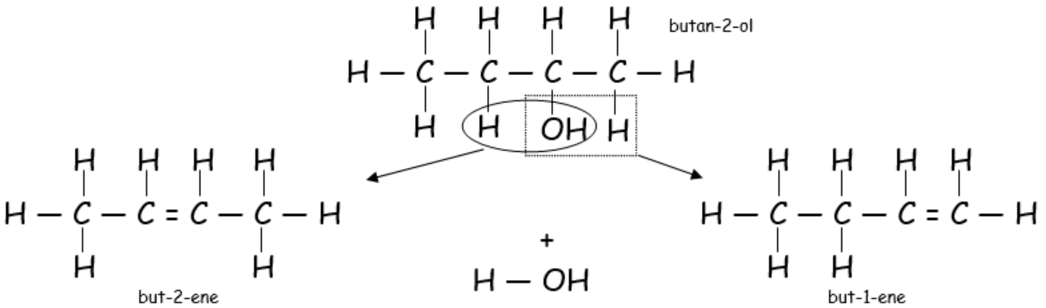
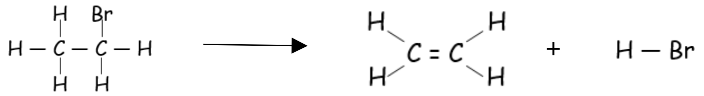
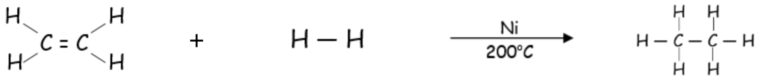
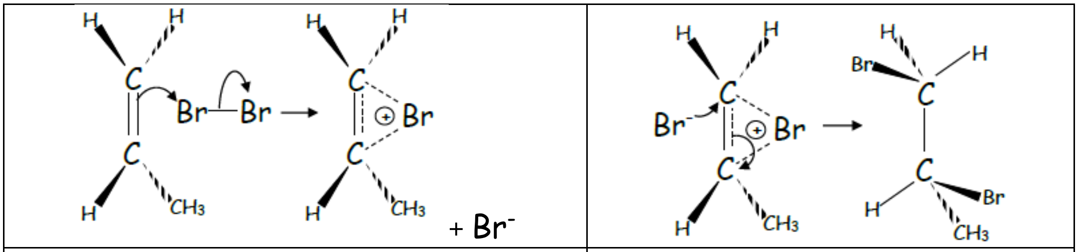
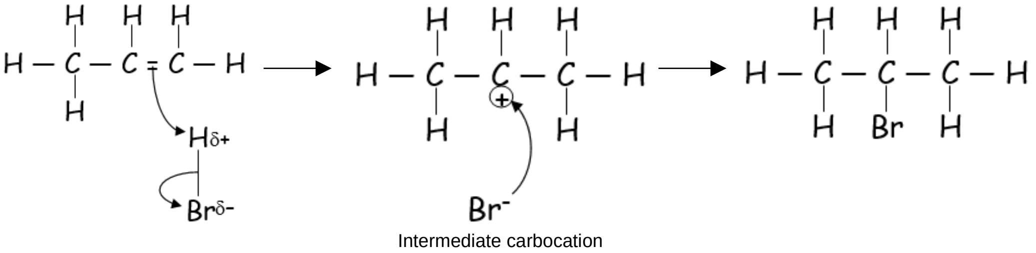
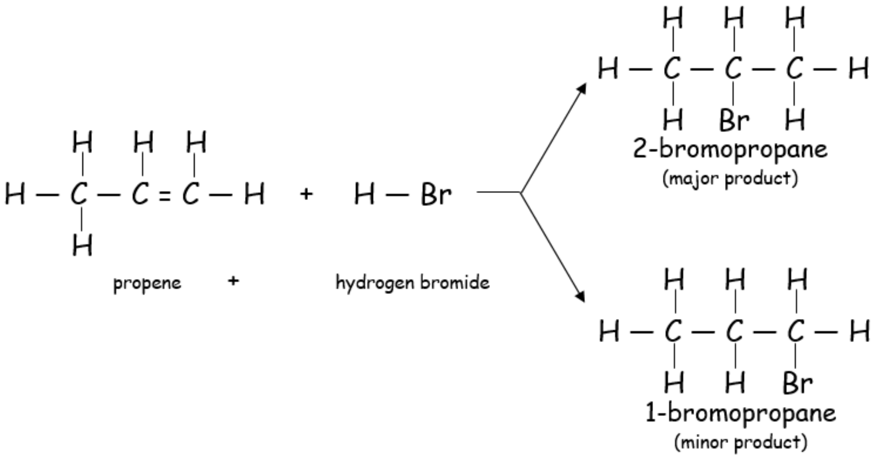
<table>
<tr><td>210</td><td>Alcohols can be oxidised by:


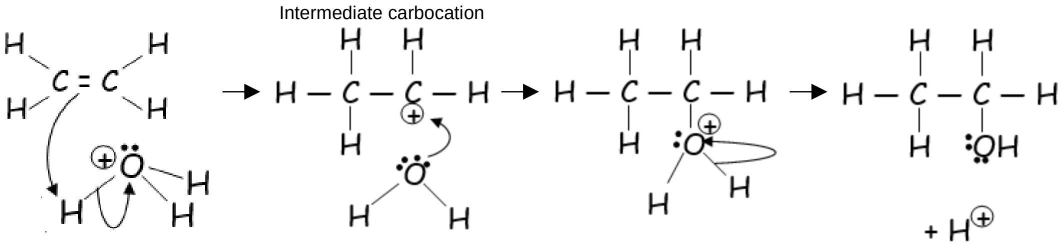
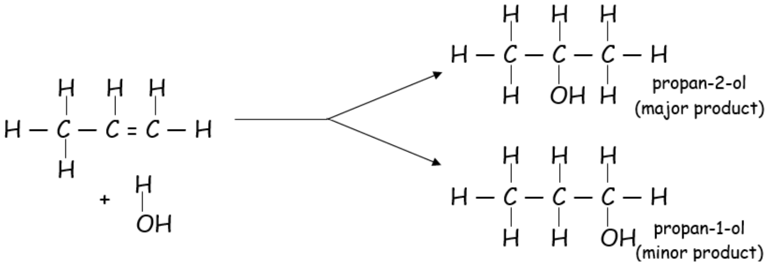
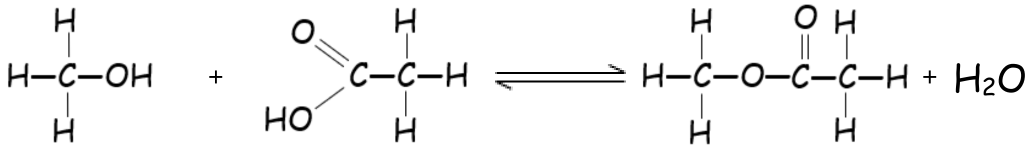
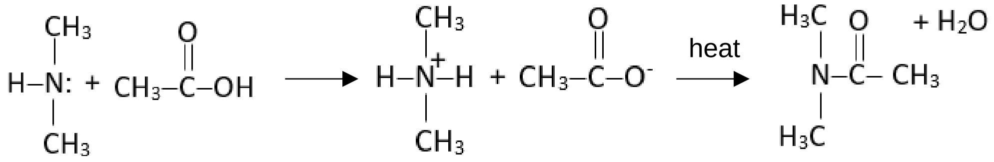
<table>
<tr><td>Oxidising Agent</td><td>acidified permanganate</td><td>acidified dichromate</td><td>hot copper (II) oxide</td></tr>
<tr><td>Colour Change</td><td>Purple→Colourless</td><td>Orange→Green</td><td>Black→Brown</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>212</td><td>Alcohols can form esters by reaction with carboxylic acids using concentrated sulfuric acid or concentrated phosphoric acid as a catalyst.

</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>213</td><td>Alcohols can form esters by reaction with acid chlorides
Faster reaction than alcohols reacting with carboxylic acids
No catalyst needed

Acid chloride

</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>214</td><td>The hydroxyl group in alcohols makes it polar
gives rise to hydrogen bonding between alcohol molecules
higher melting and boiling points, viscosity and solubility/miscibility in water.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>215</td><td>Ethers can be regarded as substituted alkanes in which a hydrogen atom is replaced with an alkoxy functional group –OR
ethers have the general structure R' – O – R'', where R' and R'' are alkyl groups.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>216</td><td>Ethers are substituted alkanes with a substituted alkoxy group
named by adding the ending ‘oxy’ to alkyl substituent to the shorter carbon chain
longer carbon chain comes second in the name of the ether
<table>
<tr><td>ethoxyethane


ethoxy- -ethane</td>
<td>ethoxypropane


ethoxy- -propane</td>
<td>methoxy-2-methylpropane


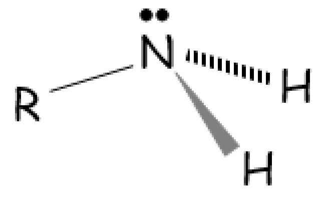
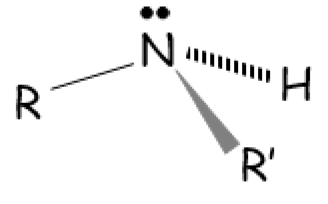
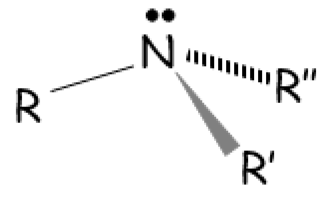
methoxy- -2-methylpropane</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>217</td><td>Ethers can be prepared in a nucleophilic substitution reaction by reacting a monohaloalkane with an alkoxide.
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>218
219
220</td><td>I know that due to the lack of hydrogen bonding between ether molecules, they have lower boiling points than the corresponding isomeric alcohols.
Ethers have lower boiling points compared to their isomeric alcohols as pure ethers lack any hydrogen bonding between molecules of ethers
methoxymethane and methoxyethane are soluble in water
larger ethers are insoluble in water due to their increased molecular size
ethers are commonly used as solvents as they are relatively chemically inert and will dissolve many organic compounds</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
</table>

221	Alkenes can be prepared by dehydration of alcohols using one from: aluminium oxide | concentrated sulphuric acid | concentrated phosphoric acid  		☹	😐	☺
222	Alkenes can be prepared by base-induced elimination of hydrogen halides from monohaloalkanes. 		☹	😐	☺
223a	Alkenes react with hydrogen to form alkanes in the presence of a catalyst by electrophilic addition reaction:  		☹	😐	☺
223b **225**	Alkenes react with halogens to form dihaloalkanes by electrophilic addition reaction:  π electrons in propene influence bond in Br_2 to split heterolytically forming the cyclic ion intermediate and Br^- ion. Br^- ion attacks cyclic ion intermediate from other side to form 1,2-dibromopropane		☹	😐	☺
223c **226a** **227a**	Alkenes react with hydrogen halides to form monohaloalkanes by electrophilic addition reactions:  • intermediate carbocation is more stable due to inductive stabilisation (FIX)		☹	😐	☺
224a	Markovikov's rule predicts major and minor products formed during the addition of hydrogen halide: • hydrogen atom in hydrogen halide adds to the C of the C=C double bonds which already has the most hydrogens attached to it  		☹	😐	☺

208b **223d** **226b** **227b**	Alkenes react with water using an acid catalyst to form alcohols by electrophilic addition reaction:  • intermediate carbocation is more stable due to inductive stabilisation (FIX)		☹	😐	☺
224b	Markovikov's rule predicts major and minor products formed during the addition of water to alkenes • hydrogen atom in water adds to the C of the C=C double bonds which already has the most hydrogens attached to it. Hydroxyl -OH group ads to other carbon in C=C  		☹	😐	☺
228	I know that carboxylic acids can be prepared by: a) oxidising primary alcohols using acidified permanganate, acidified dichromate and hot copper(II) oxide b) oxidising aldehydes using acidified permanganate, acidified dichromate, Fehling's solution and Tollens' reagent c) hydrolysing nitriles, esters or amides		☹	😐	☺
229	Carboxylic acids react with metals or bases to form salts. $2CH_3COOH + Mg \longrightarrow Mg(CH_3COO)_2 + H_2$ $CH_3COOH + NaOH \longrightarrow NaCH_3COO + H_2O$ $HCOOH + CaO \longrightarrow Ca(HCOO)_2 + H_2O$ $2C_2H_5COOH + K_2CO_3 \longrightarrow 2KC_2H_5COO + H_2O + CO_2$		☹	😐	☺
230	Carboxylic acids react with alcohols to form esters in a condensation reaction. • concentrated sulfuric or concentrated phosphoric acid present as a catalyst Alcohol + Carboxylic Acid $\rightleftharpoons$ Ester + Water  methanol + ethanoic acid $\rightleftharpoons$ methyl ethanoate + water		☹	😐	☺
231	Carboxylic acids react with amines to form alkylammonium salts that form amides when heated. e.g.  amine + carboxylic acid alkylammonium salts amide + water		☹	😐	☺
232	Carboxylic acids can be reduced with lithium aluminium hydride to form primary alcohols. e.g. butanoic acid $\xrightarrow{\text{lithium aluminium hydride}}$ butan-1-ol		☹	😐	☺

233 Amines are organic derivatives of ammonia in which one or more hydrogen atoms of ammonia has been replaced by an alkyl group. ☹ 😐 ☺

234 Amines can be classified as primary, secondary or tertiary according to the number of alkyl groups attached to the nitrogen atom. ☹ 😐 ☺

Primary Amines	Secondary Amines	Tertiary Amines
		
1 alkyl groups attached to the N atom	2 alkyl groups attached to the N atom	3 alkyl groups attached to the N atom

235 I know that amines react with acids to form salts ☹ 😐 ☺

e.g. $CH_3NH_2 + HCl \longrightarrow CH_3NH_3^+Cl^-$

236 237 Primary and secondary amines display hydrogen bonding as they contain N–H bonds. Tertiary amines do not display hydrogen bonding as they lack the N–H bond. ☹ 😐 ☺

- primary and secondary amines have higher boiling points than isomeric tertiary amines
- shorter chain length amines are more soluble in water due to hydrogen bonding

Amine	$CH_3CH_2CH_2NH_2$	$C_2H_5NHCH_3$	$(CH_3)_3N$
Type	Primary Amine	Secondary Amine	Tertiary Amine
Mass of 1mol	59g	59g	59g
Boiling Point	49°C	36°C	3°C

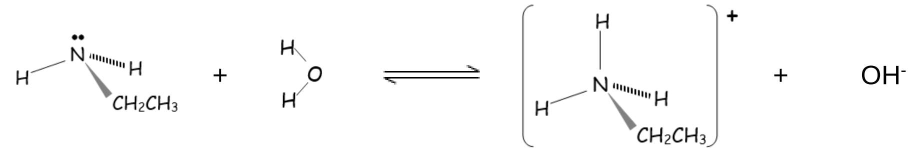
238 Amines are weak bases and dissociate to a slight extent in aqueous solution and that the nitrogen atom has a lone pair of electrons which can accept a proton (H^+) from water, producing hydroxide ions. ☹ 😐 ☺

e.g.

$$NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^-$$

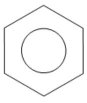
$$CH_3CH_2NH_2 + H_2O \rightleftharpoons CH_3CH_2NH_3^+ + OH^-$$

ethylamine + water ⇌ ethylammonium ion + hydroxide ion

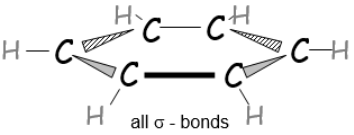
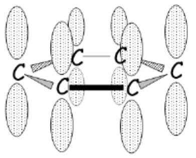
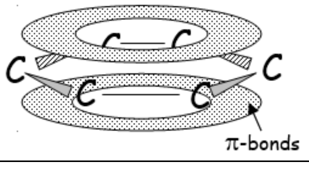


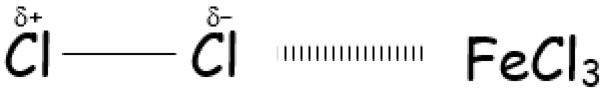
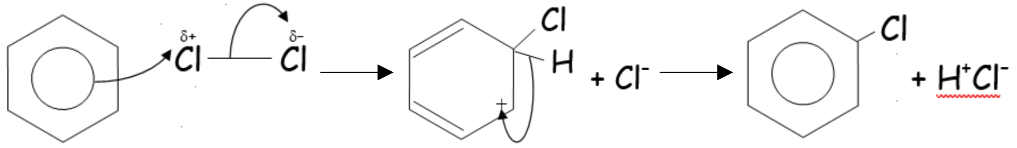
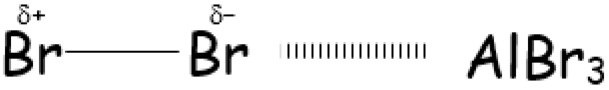
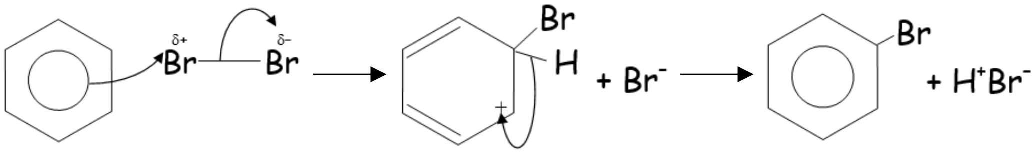
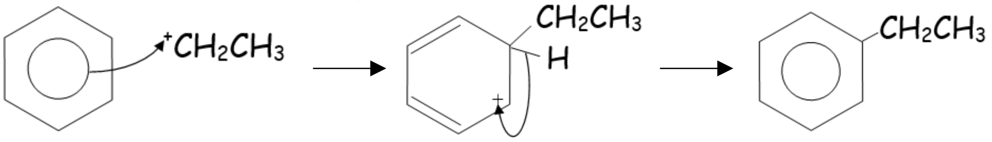
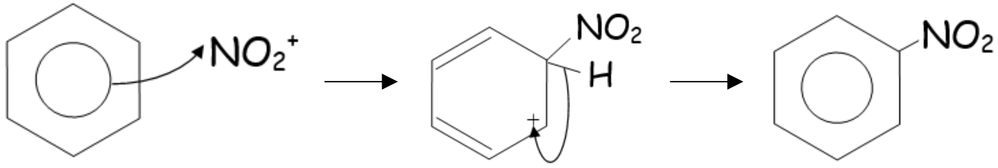
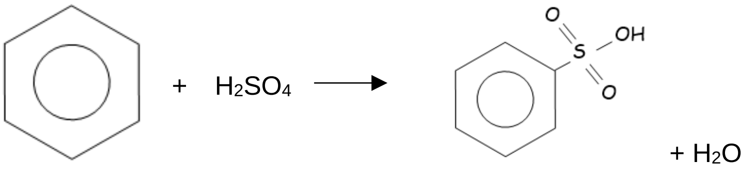
239 240 241 Benzene (C_6H_6) is the simplest member of the class of aromatic hydrocarbons. ☹ 😐 ☺

- benzene ring has a distinctive structural formula and the stability of the benzene ring is due to the delocalisation of electrons in the conjugated system
- benzene does not take part in addition reactions as there are no C=C double bonds in the structure due to the 6 delocalised electrons



242 The structure of benzene can be described in terms of sp^2 hybridiation, sigma bonds, pi bonds and electron delocalisation: ☹ 😐 ☺

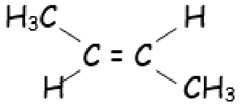
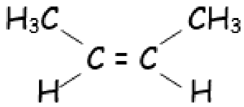
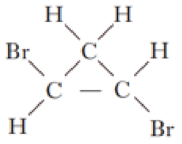
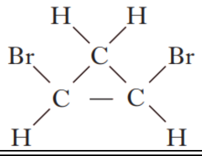
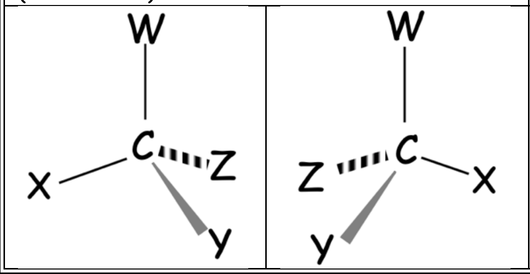
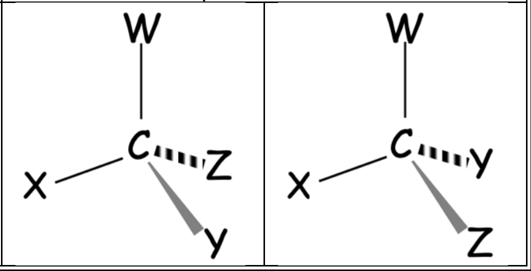
Benzene's ring structure contains sp^2 hybridisation	6 electrons not involved in sigma bonds are found in remaining six unhybridised p-orbitals	6 electrons in unhybridised p-orbitals form π–bonds
• 6 carbons and 6 hydrogen lie in same plane • 120° angle between carbons and hydrogens • all bonds shown are sigma σ-bonds	(hydrogens not drawn in diagram)	• electrons are described as delocalised • 6 electrons form 2 electron rings • stability of benzene from clouds of delocalised electrons • electron repulsion between delocalised electron rings flatten benzene structure so carbon ring becomes planar
 all σ - bonds		

243	A phenyl group is a benzene ring in which one hydrogen atom has been substituted by another group e.g. phenol C_6H_5OH, methylbenzene (toluene) $C_6H_5CH_3$ - the phenyl group has the formula $–C_6H_5$.		☹	😐	☺
244	Benzene can take part in electrophilic substitution reactions. - delocalised electrons are attractive to electrophiles for substitution reactions		☹	😐	☺
245	Benzene can undergo halogenation by reaction of a halogen - aluminium chloride or iron (III) chloride is the catalyst for chlorination where the normally non-polar Cl_2 is polarised under the influence of catalyst:  - mechanism for the electrophilic substitution reaction is:  - aluminium bromide or iron (III) bromide is the catalyst for bromination  - mechanism for the electrophilic substitution reaction is:  		☹	😐	☺
246	Benzene can undergo alkylation by reaction of a haloalkane - aluminium chloride is the catalyst for this electrophilic substitution - $AlCl_3$ catalyst causes heterolytic fission in haloalkane forming a positive electrophilic species: $CH_3CH_2Cl \xrightarrow{AlCl_3} CH_3CH_2^+ + Cl^-$ - mechanism for the electrophilic substitution reaction is:  		☹	😐	☺
247	Benzene can undergo nitration by electrophilic substitution - concentrated sulphuric acid and concentrated nitric acid react to form the electrophile nitronium NO_2^+ ion $\underset{\text{concentrated nitric acid}}{HNO_3} + \underset{\text{concentrated sulphuric acid}}{H_2SO_4} \longrightarrow \underset{\text{nitronium ion}}{NO_2^+} + \underset{\text{hydronium ion}}{H_3O^+} + \underset{\text{hydrogensulphate ion}}{2HSO_4^–}$ - nitronium NO_2^+ ion attacks the electron-rich benzene ring:  		☹	😐	☺
248	Benzene can undergo sulfonation using concentrated sulphuric acid. - SO_3 is a powerful electrophile provided by sulphuric acid  		☹	😐	☺

<table>
<tr><td></td><td colspan="2">

AH Chemistry: Organic Chemistry

Section 3c: Stereochemistry

JAB chem</td><td colspan="3">Traffic Light</td></tr>
<tr><td></td><td colspan="2"></td><td>red</td><td>amber</td><td>green</td></tr>
<tr><td>249
250</td><td>Isomers are molecules with the same molecular formula but different structural formulae.
structural isomers occur when atoms are bonded together in a different order in each isomer.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>251
252</td><td>Stereoisomers occur when the order of the bonding in the atoms is the same but the spatial arrangement of the atoms is different in each isomer.
There are two types of stereoisomer: a) geometric b) optical.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>253a
254a
255a</td><td>Geometric isomers occur when there is restricted rotation around a C=C double bond.
two different groups attached to each carbon atom that makes up the C=C bond
CIS isomer if both groups are on the SAME side of C=C
TRANS isomer if both groups are on the SAME side of C=C
<table>
<tr><td>trans-but-2-ene</td><td>cis-but-2-ene</td></tr>
<tr><td></td><td></td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>253b
254b
255b</td><td>Geometric isomers occur when there is restricted rotation around a carbon-carbon single bond in a cyclic compound.
two different groups attached to each carbon atom that makes up the C–C bond
CIS isomer as both groups are on the SAME side of restricted C–C bond in the ring structure
TRANS isomer as both groups are on the SAME side of restricted C–C bond in the ring structure
<table>
<tr><td>trans-1,2-dibromocyclopropane</td><td>cis-1,2-dibromocyclopropane</td></tr>
<tr><td></td><td></td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>256</td><td>Geometric isomers have differences in physical properties e.g. melting and boiling points
<table>
<tr><th>Geometric Isomer</th><th>Melting Point (^oC)</th><th>Boiling Point (^oC)</th></tr>
<tr><td>cis-but-2-ene</td><td>-139</td><td>+4</td></tr>
<tr><td>trans-but-2-ene</td><td>-106</td><td>+1</td></tr>
</table>
Geometric isomers and can have differences in chemical properties.
e.g. cis-but-2-enedioic acid undergoes dehydration reactions but trans-but-2-enedioic acid as in the trans isomer the carboxyl groups are pointing away from each other</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>257
259</td><td>Optical isomers occur in compounds which have four different groups arranged tetrahedrally around a central carbon atom (chiral carbon or chiral centre).
optical isomers can be described as enantiomers.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>258</td><td>Optical isomers are asymmetric, non-superimposable mirror images of each other.
<table>
<tr><td><u>Non-superimposable Mirror Images</u>
Images shown are direct mirror images of each other and are therefore are optical isomers (enantiomers)</td><td><u>Non-superimposable Mirror Images</u>
The following are optical isomers as Groups W and X are in the same position but Groups Y and Z are in different position.</td></tr>
<tr><td> </td><td> </td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>260
261
262</td><td>Optical isomers have identical physical properties except for their effect on plane-polarised light.
optical isomers are optically active as they rotate plane-polarised light by the same amount but in opposite directions
Optical isomers have identical chemical properties, except when in a chiral environment such as that found in biological systems where only one optical isomer is usually present.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>263</td><td>A racemic mixture is when optical isomers are mixed in equal amounts and is optically <u>in</u>active
rotational effect of the plane-polarised light cancels out and called a racemic mixture.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
</table>

AH Chemistry: Inorganic Chemistry

Section 3d: Experimental Determination of Structure

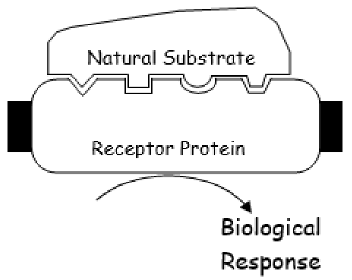
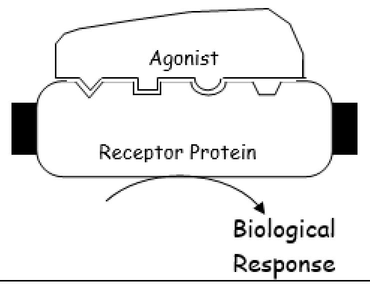
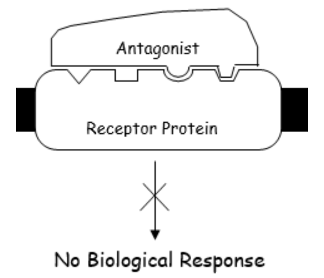
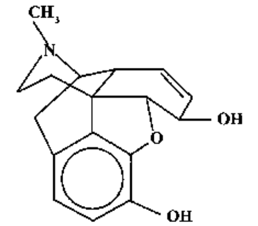
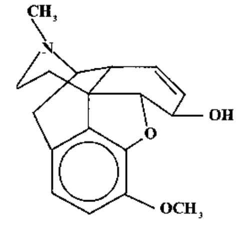
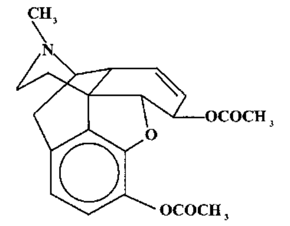
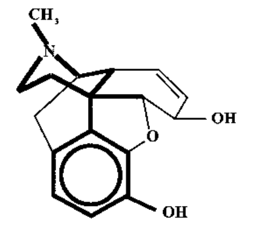
JAB chem

			Traffic Light		
			red	amber	green
264 265	I know that elemental microanalysis is used to determine the masses of C, H, O, S and N in a sample of an organic compound in order to determine its empirical formula. I know that an empirical formula shows the simplest ratio of the elements in a molecule.		☹	😐	☺
266 267	I can determine an empirical formula from elemental microanalysis data. I know that elemental microanalysis can be determined from: • combustion product masses • percentage product by mass		☹	😐	☺
268	I know that mass spectrometry can be used to determine the accurate gram formula mass (GFM) and structural features of an organic compound.		☹	😐	☺
269 270	I know in mass spectrometry, a small sample of an organic compound is bombarded by high-energy electrons and this removes electrons from the organic molecule generating positively charged molecular ions known as parent ions. I know that the molecular ions then break into smaller positively charged ion fragments and a mass spectrum is obtained showing a plot of the relative abundance of the ions detected against the mass-to-charge (m/z) ratio.		☹	😐	☺
281 282	I can use mass-to-charge ratio of the parent ion to determine the GFM of the molecular ion, and determine a molecular formula using the empirical formula. I know that the fragmentation data from mass spectrometry can be interpreted to gain structural information.		☹	😐	☺
283 284	I know that Infrared spectroscopy is used to identify certain functional groups in an organic compound. I know that when infrared radiation is absorbed by organic compounds, bonds within the molecule vibrate (stretch and bend) and the wavelengths of infrared radiation that are absorbed depend on the type of atoms that make up the bond and the strength of the bond.		☹	😐	☺
285 286 287	I know that in infrared spectroscopy, infrared radiation is passed through a sample of the organic compound and then into a detector that measures the intensity of the transmitted radiation at different wavelengths. I know that the absorbance of infrared radiation is measured in wavenumbers, the reciprocal of wavelength, in units of cm^{-1}. I know characteristic absorptions by particular vibrations are given in the data booklet.		☹	😐	☺
288	I can interpret infrared spectra.		☹	😐	☺
289	I know that proton nuclear magnetic resonance spectroscopy (proton NMR or ^{1}H NMR) can give information about the different chemical environments of hydrogen atoms (protons or ^{1}H) in an organic molecule, and about how many hydrogen atoms there are in each of these environments. I can explain how ^{1}H nuclei emit radiation that can be plotted on a spectrum		☹	😐	☺
291 292 293 294	I know that In a ^{1}H NMR spectrum the chemical shift, δ , (peak position) is related to the environment of the ^{1}H atom and is measured in parts per million (ppm). I know that chemical shift values for ^{1}H in different chemical environments are given in the data booklet I know that the area under the peak is related to the number of ^{1}H atoms in that environment and is often given by an integration curve on a spectrum. I know that the height of an integration curve is proportional to the number of ^{1}H atoms in that environment, and so a ratio of ^{1}H atoms in each environment can be determined.		☹	😐	☺
295	I know that the standard reference substance used in ^{1}H NMR spectroscopy is tetramethylsilane (TMS), which is assigned a chemical shift value equal to zero.		☹	😐	☺
296 297	I know that ^{1}H NMR spectra can be obtained using low-resolution or high-resolution NMR. I know that high-resolution ^{1}H NMR uses higher radio frequencies than those used in low-resolution ^{1}H NMR and provides more detailed spectra.		☹	😐	☺
298 299	I know that in a high-resolution ^{1}H NMR an interaction with ^{1}H atoms on neighbouring carbon atoms can result in the splitting of peaks into multiplets. I know that the number of ^{1}H atoms on neighbouring carbon atoms will determine the number of peaks within a multiplet and can be determined using the n+1 rule, where n is the number of ^{1}H atoms on the neighbouring carbon atom.		☹	😐	☺
300	I can analyse low- and high-resolution ^{1}H NMR spectra, and can sketch low-resolution ^{1}H NMR spectra for any given compound.		☹	😐	☺

AH Chemistry: Inorganic Chemistry

Section 3e: Pharmaceutical Chemistry

JAB chem

			Traffic Light		
			red	amber	green
301 **302** **303**	Drugs are substances that alter the biochemical processes in the body. • drugs that have beneficial effects are used in medicines. • medicines usually contain the drug plus other ingredients such as fillers to add bulk or sweeteners to improve the taste.		☹	😐	☺
304	Drugs generally work by one of two mechanisms: • binding to specific protein molecules found on the surface of a cell. The protein molecules which the drug fits into is called a receptor. • binding to specific enzyme molecules within a cell.		☹	😐	☺
305 **306** **307**	I know that drugs that act on receptors can be classified as agonists or antagonists. • an agonist molecule mimics the body's naturally active compound(s) and binds to the receptor molecules to produce a similar biological response to the natural active compound. e.g. asthma medicine salbutamol stimulates receptors for adrenaline in the airways to open the airways during an asthma attack • an antagonist molecule prevents the body's naturally active compound(s) from binding to the receptor and blocks the body's naturally chemicals from interacting with that receptor e.g. atenolol is a beta blocker drug for slowing heart rate as it is an antagonist drug for the adrenaline receptor in the heart. Adrenaline in the body then cannot bind with that receptor preventing any adrenaline speeding up the heart rate. Natural Substrate  Agonist  Antagonist  		☹	😐	☺
308	Many drugs that act on enzymes are classified as enzyme inhibitors • act by binding to the active site of the enzyme • block the reaction normally catalysed by the enzyme		☹	😐	☺
309 **310**	The receptor binding site or active site in an enzyme interacts with the drug and the interaction is specific to the size and shape of the drug. • different types of van der Waals forces and ionic forces are involved in the interaction from the drug to the receptor/enzyme. • the structural fragment of a drug molecule that allows it to form interactions with a receptor binding site/enzyme active site normally consists of different functional groups correctly orientated with respect to each other.		☹	😐	☺
311	The structures of drugs that have similar effects on the body can be analysed and the structural fragment can be identified that is involved in the drug action.  morphine  codeine  diamorphine  common shape		☹	😐	☺

AH Chemistry: Researching Chemistry

Section 4a: Common Chemical Apparatus

JAB chem

Traffic Light: red, amber, green

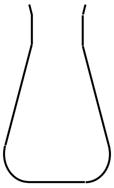
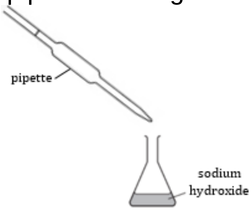
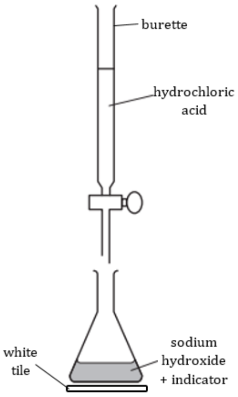
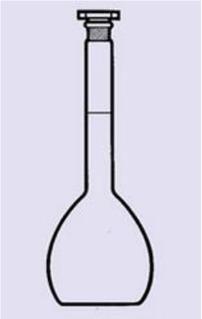
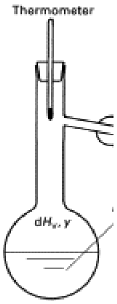
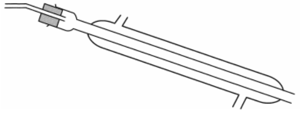
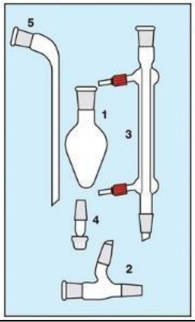
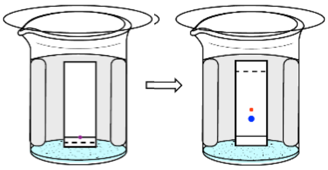
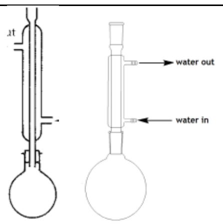
312

I am familiar with the following apparatus:

a) Conical Flask	b) digital balance	c) pipette with digital filler
d) burette	e) volumetric (standard) flask	f) distillation (round bottom) flask
g) condenser	h) thermometer	i) Buchner Funnel
j) Quick Fit Glassware	k) thin layer chromatography	l) colorimetry
m) melting point apparatus	n) separating funnel	

☹ 😐 ☺

312

a) Conical Flask  Conical flasks are used in titrations because their shape allows the swirling of the contents without spillage	b) digital balance 	c) pipette with digital filler 
d) burette  	e) volumetric (standard) flask 	f) distillation (round bottom) flask 
g) condenser 	h) thermometer  Used to measure temperature. Make sure end of thermometer is still in the substance you measuring temperature of.	i) Buchner Funnel 
j) Quick Fit Glassware  	k) thin layer chromatography 	l) colorimetry 
m) melting point apparatus 	n) separating funnel 	

☹ 😐 ☺

AH Chemistry: Researching Chemistry

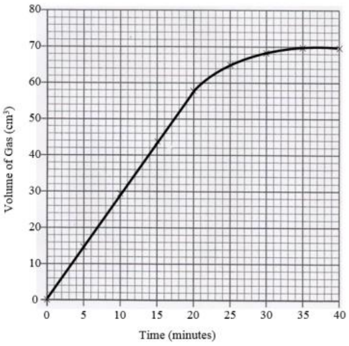
Section 4b: Skills Involved in Practical Work

Traffic Light: red amber green

313a
313b
313c

Data can be tabulated using appropriate headings and units of measurement
Data can be represented as a scatter graph with suitable scales and labels.
A straight or curved line of best fit can be drawn to represent the trend observed in the data.

Time (minutes)	Volume of Gas (cm³)
0	0
5	14
10	28
15	44
20	58
25	65
30	68
35	70
40	70



☹ 😐 ☺

313d
313e

Average (mean) values can be calculated from raw data.

- The first (rough) titre should be excluded from the calculation of the average value
- Rogue points should be identified and eliminated from calculation of the averages

Titration	Start Volume (cm³)	Final Volume (cm³)	Change in Volume (cm³)
1	0.0	11.4	11.4
2	11.4	21.7	10.3
3	21.7	36.2	14.5
4	36.2	46.7	10.5

$$\text{Average Volume} = \frac{10.3 + 10.5}{2} = \frac{20.8}{2} = 10.4\text{cm}^3$$

☹ 😐 ☺

313f

The relative accuracy of apparatus used to measure the volume of liquids can be commented on:

Beaker	Measuring Cylinder	Pipette	Burette
Beakers are of little use in measuring the volume of liquids accurately and only provide a rough guide to the volume.	Measuring Cylinders have often used to measuring volumes and the accuracy is ±0.5cm³ (i.e. half the smallest division on the measuring cylinder)	Pipettes (used with a pipette filler) give much more accurate volumes than measuring cylinders with accuracy like ±0.06cm³ typical in a 25cm³ pipette.	Burettes are used for measuring non-standard volumes of liquid but are not as accurate as a pipette as the error from the top reading is added to the error at the bottom reading of the scale.

☹ 😐 ☺

313g

The reproducibility of results where measurements have been made can be commented on:

Accurate
Precise

Not Accurate
Precise

Accurate
Not Precise

Not Accurate
Not Precise

☹ 😐 ☺

313h

Quantitative stoichiometric calculations can be performed:

no. of mol thiosulphate = **v**olume x **c**oncentration = 0.0205 x 0.10 = 0.00205 mol

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

2mol 1mol
0.00205mol 0.001025mol

$$ClO^- \quad + \quad 2I^- \quad + \quad 2H^+ \longrightarrow I_2 \quad + \quad Cl^- \quad + \quad H_2O$$

1mol 1mol
0.001025mol 0.001025mol

no. of mol of ClO^- ions in 25cm³ of solution = 0.001025mol
no. of mol of ClO^- ions in 250cm³ of solution = 0.01025mol

$$\textbf{c}\text{oncentration} = \frac{\textbf{n}\text{o. of mol}}{\textbf{v}\text{olume}} = \frac{0.01025 \text{ mol}}{0.010 \text{ litres}} = 1.025\text{mol l}^{-1}$$

☹ 😐 ☺

313i

Spectral data can be analysed for:

Mass Spectrometry (Section 3d Outcomes 269-282)	IR Spectroscopy (Section 3d Outcomes 283-288)	Proton NMR Spectroscopy (Section 3d Outcomes 289-300)	Absorption Spectroscopy (Section 1a Outcomes 17-18)

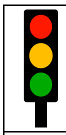
☹ 😐 ☺

313j

A control experiment can be completed in a practical validate a technique or procedure as accurate.
e.g. In the quantitative analysis of vitamin C in orange juice

- the accuracy of the measurement of vitamin C in orange juice can be checked by using a pure vitamin C solution known concentration.
- repeat the practical to check the concentration calculated in the practical is accurate against the known concentration of the control experiment.

☹ 😐 ☺



AH Chemistry: Researching Chemistry

Section 3c: Stoichiometric Calculations

JAB chem

Traffic Light: red | amber | green

314
315

Stoichiometry is the study of mole relationships involved in chemical reactions.

- Chemical equations can be written and balanced
- State symbols used for solid (s), liquid (l), gas (g) and aqueous (aq)
- Mole ratios can be used to work out quantities of other reactants or products

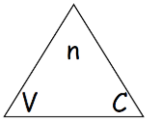
$$CaCO_{3(s)} + 2HCl_{(aq)} \longrightarrow CaCl_{2(aq)} + H_2O_{(l)} + CO_{2(g)}$$

$CaCO_{3(s)}$	$2HCl_{(aq)}$
1mol	2mol
0.1mol	0.2mol

☹ 😐 ☺

316b
316c
316d
320d

For solutions, the number of moles, the volume of solution or the concentration of a solution can be calculated from the other quantities.



n= number of moles (mol)
V = volumes (l)
C = concentration (mol l^{-1})

Calculate the number of moles of solute dissolved in 200cm^3 of 0.1 mol l^{-1} solution.	Calculate the concentration of solute if 0.5mol is dissolved in 400cm^3 of solution.	Calculate the volume of solution where 0.1mol of solute is dissolved and the concentration is 0.02mol l^{-1}.
n = ? V = 0.2 litres C = 0.1mol l^{-1} n = V x C = 0.2 litres x 0.1 mol l^{-1} = 0.02 mol	n = 0.5mol V = 0.4 litres C = ? $C = \frac{n}{V} = \frac{0.5}{0.4} = 1.25$ mol l^{-1}	n = 0.1mol V = ? C = 0.02mol l^{-1} $V = \frac{n}{C} = \frac{0.1}{0.02} = 5$ mol l^{-1}

☹ 😐 ☺

320a

Gram formula mass (GFM) is calculated from the formula and Relative Atomic Mass:
e.g.: Calculate the gfm of calcium nitrate:
gfm $Ca(NO_3)_2$ = (1x40.1) + (2x14) + (6x16) = 40.1 + 28 + 96 = 164.1 g mol^{-1}

☹ 😐 ☺

320b
320c

Calculations turning masses into number of moles (and vice versa) require the gfm:

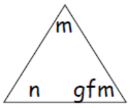
Calculate the number of moles in 0.328g of calcium nitrate?	Calculate the mass of 0.05mol of calcium nitrate?
gfm $Ca(NO_3)_2$ =164.1g mol^{-1} **n**o. of mol = $\frac{\textbf{mass}}{\textbf{gfm}} = \frac{0.328}{164.1}$ = 0.002mol	gfm $Ca(NO_3)_2$ =164.1g mol^{-1} **m**ass = **n**o. of mol x **gfm** = 0.05 x 164.1 = 8.21g

☹ 😐 ☺

316a

The mass of solute in solutions can be calculated.

e.g. calculate the mass of sodium oxide dissolved in 200cm^3 or 0.025mol l^{-1} solution.



m = mass (g)
n= number of moles (mol)
gfm = gram formula mass (g mol^{-1})

gfm Na_2O = (2x23) + (1x16) = 46 + 16 = 62g mol^{-1}	n = ? V = 0.2 litres C = 0.025mol l^{-1} n = V x C = 0.2 litres x 0.025 mol l^{-1} = 0.05 mol	m = ? n = 0.5mol gfm = 62g mol^{-1} m = n x gfm = 0.05 mol x 62g mol^{-1} = 3.1g

☹ 😐 ☺

317

Percentage by mass is the mass of solute made up to 100 cm^3 of solution.

- a 1% starch indicator solution contains 1g of starch dissolved deionised water and the solution made up to 100cm^3 with deionised water.

☹ 😐 ☺

318

Percentage by volume is the number of cm^3 of solute made up to 100 cm^3 of solution.

- A 10% ethanol solution contains 10cm^3 of ethanol and the solution made up to 100cm^3 with deionised water.

☹ 😐 ☺

319

The unit ppm stands for parts per million and refers to 1 mg per kg or 1 mg per litre.

The steel from a sword blade of mass 1300 g was found to have a vanadium concentration of 71 ppm. Calculate the total mass of vanadium present in the sword blade.	An adrenaline dose contains 0·3 cm^3 of 500 ppm adrenaline solution. Calculate the mass of adrenaline, in mg, delivered in one dose.
71ppm = 71mg Vanadium in 1kg steel 1kg steel contains 71mg Vanadium 1000g steel contains 71mg Vanadium 1300g steel contains 71mg Vanadium x $^{1300}/_{1000}$ = 92.3mg Vanadium	500ppm = 500mg per litre 1 litre contains 500mg adrenaline 1000cm^3 contains 500mg adrenaline 0.3cm^3 contains 500mg adrenaline x $^{0.3}/_{1000}$ = 0.15mg adrenaline

☹ 😐 ☺

320e

Calculations using volumes of gases include:

Calculate the final volume and composition when 10cm^3 of butane gas is completely burned in 100cm^3 of oxygen. All measurements made at the same temperature and pressure.	Calculate the volume of carbon dioxide formed when 2g of calcium carbonate is reacted with excess hydrochloric acid. Molar volume = 24litres
$C_4H_{10(g)} + 6\frac{1}{2}O_{2(g)} \rightarrow 4CO_{2(g)} + 5H_2O_{(l)}$ 1mol 6.5mol 4mol 5mol 1vol 6.5vol 4vol negligible vol 10cm^3 65cm^3 40cm^3 - + 35cm^3 leftover Final Volume = 75cm^3 (40cm^3 CO_2 + 35cm^3 O_2)	gfm $CaCO_3$ = (1x40.1)+(1x12)+(3x16) = 100.1g **n**o. of mol = $\frac{\textbf{mass}}{\textbf{gfm}} = \frac{2}{100.1}$ = 0.02mol $CaCO_3 + 2HCl \rightarrow CaCl_2 + H_2O + CO_2$ 1mol 1mol 0.02mol 0.02mol **V**olume = **n**o. of mol x **M**olar **V**olume = 0.02 x 24 = 0.48litres

☹ 😐 ☺

<table>
<tr><td>320f</td><td>Calculations can be done to calculate reactant excess:
e.g. Calculate the reactant which is the limiting factor and which reactant is in excess when 6g of calcium carbonate reacts with 50cm^3 of 0.5mol l^{-1} hydrochloric acid.
gfm $CaCO_3$ = (1x40.1)+(1x12)+(3x16) = 100.1g
HCl no. of mol = volume x concentration
= 0.05$_{\text{litres}}$ x 0.5 mol l^{-1}
= 0.025mol (available)
no. of mol = $\dfrac{\textbf{m}\text{ass}}{\textbf{gfm}} = \dfrac{6}{100.1}$ = 0.060mol
$$\underset{\substack{\text{1mol}\\ \text{0.060 mol}}}{CaCO_3} + \underset{\substack{\text{2mol}\\ \text{0.120mol}\\ \text{(needed)}}}{2HCl} \rightarrow CaCl_2 + H_2O + CO_2$$
0.060mol of $CaCO_3$ needs 0.120mol of HCl to fully react but only 0.025mol $CaCO_3$ is available ∴ HCl is the limiting factor and $CaCO_3$ is in excess.
Alternately
$$\underset{\substack{\text{1mol}\\ \text{0.050mol}\\ \text{(needed)}}}{CaCO_3} + \underset{\substack{\text{2mol}\\ \text{0.025mol}}}{2HCl} \rightarrow CaCl_2 + H_2O + CO_2$$
0.025mol of HCl needs 0.050mol of $CaCO_3$ to fully react. 0.060mol $CaCO_3$ is available ∴ HCl is the limiting factor and $CaCO_3$ is in excess.</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>320h</td><td>Empirical Formula is worked out from mass or percentages of each element in compound.
e.g. Calculate the empirical formula when 5·00 g of an organic compound was burned completely producing 11·89 g of CO_2 and 6·08 g of H_2O as the only products.
• Mass of carbon in CO_2 = $^{12}/_{44}$ x 11.89g = 3.243g
• Mass of hydrogen in H_2O = $^{2}/_{18}$ x 6.08g = 0.676g
• Mass of oxygen = 5g – (3.243+0.676) = 5 – 3.919 = 1.081g
<table>
<tr><th>Elements</th><th>C</th><th>H</th><th>O</th><th></th></tr>
<tr><td>Mass or %</td><td>3.243g</td><td>0.676g</td><td>1.081g</td><td></td></tr>
<tr><td>Divide by RAM</td><td>$\frac{3.243g}{12g\ mol^{-1}}$
= 0.270mol</td><td>$\frac{0.676g}{1g\ mol^{-1}}$
= 0.676mol</td><td>$\frac{1.081g}{16g\ mol^{-1}}$
= 0.0676mol</td><td></td></tr>
<tr><td>Divide through by smallest number</td><td>$\frac{0.270mol}{0.0676mol}$
= 4</td><td>$\frac{0.676mol}{0.0676mol}$
= 10</td><td>$\frac{0.0676mol}{0.0676mol}$
= 1</td><td></td></tr>
<tr><td>Empirical Formula</td><td>4</td><td>10</td><td>1</td><td>$C_4H_{10}O$</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>320g
321</td><td>Percentage Yield can be calculated from actual yield and theoretic yield.
e.g. Calculate the percentage yield if 20kg of ammonia is formed from 12kg of hydrogen reacting with excess nitrogen.
$$N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)}$$
3mol 2mol
6g 34g
12g 68g
12kg 68kg (theoretical yield)
$$\text{\% Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \text{x100} = \frac{20kg}{68kg} \text{x100} = 29.4\%$$</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>322</td><td>The percentage yield actually achieved in a process is reduced by:
<table>
<tr><td>mass transfer or mechanical losses</td><td>purification of product</td><td>side reactions</td><td>equilibrium position</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
</table>

AH Chemistry: Researching Chemistry

Section 4d: Gravimetric Analysis

JAB chem

			Traffic Light		
			red	amber	green
323 **324**	Gravimetric analysis can determine the mass of an element or compound in a substance. • an accurate electronic balance can be used to determine the mass of substance ○ the tare function on the balance allows the balance to be set to zero when an object is on top of the balance pan • weighing boats are used to measure substances on a balance without contamination • weighing by difference is used to accurately measure the mass of substance. ○ The mass of an empty weighing bottle and stopper is measured and the chemical is added to the bottle and reweighed. The difference is the mas of the substance in the bottle. • 'weighing accurately approximately' is the term used to measure the exact mass of a substance on a balance but the mass is close to a specific mass stated ○ Weigh accurately approximately 2g of substance should mean that a mass was added close to 2.00g and was accurately measured to be 2.02g. • heating to constant mass is used to remove all moisture from a substance which would increase the mass of the substance ○ The substance is heated to remove moisture from the substance. ○ The substance is allowed to cool in a desiccator to prevent reabsorption of water ○ The substance has its mass measured on the balance once cooled. ○ Repeating the steps of heating, cooling and weighing until constant mass is obtained on the balance.		☹	😐	☺
325a **326**	Conversion of the substance can occur when the substance undergoes a precipitation reaction to allow isolation and purification. • The precipitate is separated from the filtrate • the filtrate tested to ensure the reaction has gone to completion. • the precipitate is washed, dried to constant mass and then weighed.		☹	😐	☺
325b **327**	Conversion of the substance can also be achieved by volatilisation to allow isolation and purification. • the substance is heated and any volatile products (often water) are evaporated. • the substance is heated to constant mass and the final mass recorded.		☹	😐	☺

AH Chemistry: Researching Chemistry

Section 4e: Volumetric Analysis

JAB chem

			Traffic Light		
			red	amber	green
328	I am familiar with use of the technique of volumetric analysis, including: • preparing a standard solution • accurate dilution • standardising solutions to determine accurate concentration • titrating to obtain concordancy using burettes, pipettes and volumetric flasks • choosing an appropriate indicator		☹	😐	☺
329	A standard solution is a solution of accurately known concentration.		☹	😐	☺
330	Standard solutions can be prepared by: • weighing a primary standard accurately • dissolving in a small volume of solvent (usually deionised/distilled water) in a beaker • transferring the solution and rinsings into a volumetric flask • making up to the graduation mark with solvent stoppering and inverting		☹	😐	☺
331	Standard solutions can be prepared by accurate dilution • pipette an appropriate volume of a standard solution into a volumetric flask • make up to the graduation mark with solvent (water), stoppering and inverting.		☹	😐	☺
332	Primary standards must have the following properties: high state of purity stable when solid and in solution soluble reasonably high GFM		☹	😐	☺
333	Examples of primary standards include: sodium carbonate Na_2CO_3 hydrated oxalic acid $H_2C_2O_4{\cdot}2H_2O$ potassium hydrogen phthalate $KH(C_8H_4O_4)$ silver nitrate $AgNO_3$ potassium iodate KIO_3 potassium dichromate $K_2Cr_2O_7$		☹	😐	☺
334 **335**	Sodium hydroxide cannot be used as a primary standard: a relatively low GFM unstable as a solid (absorbs moisture) unstable as a solution • Sodium hydroxide solution must be standardised before being used in volumetric analysis.		☹	😐	☺
336	Acid-base titrations are used for volumetric analysis between acids and bases. e.g. Calculate the number of moles of sulphuric acid which reacts with 14.7cm^3 of 0.5mol l^{-1} NaOH solution. **n**o. of mol = **v**olume x **c**oncentration = 0.0147 litres x 0.5mol l^{-1} = 0.00735mol $\begin{array}{ccccccc} H_2SO_4 & + & 2NaOH & \rightarrow & Na_2SO_4 & + & 2H_2O \\ 1mol & & 2mol & & 1mol & & 2mol \\ 0.00735mol & & \underline{0.01470mol} & & & & \end{array}$		☹	😐	☺
337	Redox titrations are used for volumetric analysis between oxidising and reducing agents: e.g. Calculate the number of moles of ethanol which reacts with 22.4cm^3 of 0.02mol l^{-1} dichromate solution. **n**o. of mol = **v**olume x **c**oncentration = 0.0224 litres x 0.02mol l^{-1} = 0.000448mol $\begin{array}{ccccccccccc} 3C_2H_5OH & + & 2Cr_2O_7^{2-} & + & 16H^+ & \rightarrow & 3CH_3COOH & + & 4Cr^{3+} & + & 11H_2O \\ 3mol & & 2mol & & & & & & & & \\ \underline{0.000672mol} & & 0.000448mol & & & & & & & & \end{array}$		☹	😐	☺
338	Complexometric titrations are based on reactions using complexometric reagents like E.D.T.A. to form complexes with metal ions to determine the concentration of metal ions. e.g. Calculate the number of moles of Ni$^+$ that reacts with 23.05cm^3 of 0.01 mol l^{-1} E.D.T.A **n**o. of mol = **v**olume x **c**oncentration = 0.02305 litres x 0.01mol l^{-1} = 0.0002305mol $\begin{array}{ccccc} E.D.T.A & + & Ni^{2+} & \rightarrow & Ni^{2+} / E.D.T.A.\ Complex \\ 1mol & & 1mol & & 1mol \\ 0.0002305mol & & \underline{0.0002305mol} & & \end{array}$		☹	😐	☺
339 **340** **341**	Back titrations are used to find the number of moles of a substance by reacting it with an excess volume of a reactant of known concentration. • An excess of a known reactant (e.g. *standardised hydrochloric acid*) is added to the unknown reactant (e.g. *calcium carbonate*) and allowed to fully react. • The unreacted leftover reactant (e.g. *hydrochloric acid*) is then titrated against another chemical (e.g. *standardised sodium hydroxide*) to calculate the number of moles of known reactant that was left over. • The number of moles of known reactant (e.g. *hydrochloric acid*) which reacted with the unknown chemical (e.g. *calcium carbonate*) is calculated by subtracting the number of moles of known reactant leftover (e.g. *hydrochloric acid*) from the number of moles at the start. • The initial number of moles of the unknown substance (e.g. *calcium carbonate*) is then calculated using stoichiometry in a balanced chemical equation. • back titrations are useful when working out the quantity of substance in a solid with a low solubility.		☹	😐	☺

<table>
<tr><th rowspan="2"></th><th rowspan="2"><h1>AH Chemistry: Researching Chemistry</h1><h2>Section 4f: Practical Skills & Techniques</h2>JAB chem</th><th rowspan="2"></th><th colspan="3">Traffic Light</th></tr>
<tr><th>red</th><th>amber</th><th>green</th></tr>
<tr><td>342</td><td>Colorimetry can be used to measure the concentration of a species based on its absorbance of a particular wavelength of light. It involves:

preparing a series of standard solutions of an appropriate concentration
choosing an appropriate colour or wavelength of filter complementary to the colour of the species being tested using a blank
preparing a calibration graph
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>343
344
345
346</td><td>Colorimetry uses the relationship between colour intensity of a solution and the concentration of the coloured species present.

The higher the concentration of the species the higher the absorbance of light
colorimeter (spectrophotometer) measures the absorbance of light of a series of standard solutions
absorbance data is used to plot a calibration graph against concentration
solutions with unknown concentration are tested the absorbance obtained can determine the concentration of the species on the calibration curve.
the solution of unknown concentration must have an absorbance that must lie in the straight line section of the calibration graph.
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>347
348
349</td><td>Distillation is used for identification and purification of organic compounds

the boiling point of a compound can be determined by distillation
boiling point is one of the physical properties which can identify compounds
the more volatile compound (with the lower boiling point) is separated from the less volatile compound and can purify the more volatile compound.
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>350
351
352</td><td>Heating under reflux allows heat energy to be applied to a chemical reaction mixture over an extended period of time without volatile substances escaping.

reaction mixture is placed in a round-bottomed flask with anti-bumping granules
flask is fitted with a condenser (water goes in end of condenser nearest round bottom flask)
flask is heated using appropriate source of heat. (heating mantle for flammable liquids)
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>353
354
355</td><td>Vacuum filtration involves carrying out a filtration under reduced pressure and provides a faster means of separating a precipitate from a filtrate.

The following can be used for vacuum filtration using a suction pump to help speed up the time taken for the filtration to take place.:

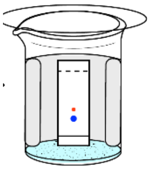
<table>
<tr><td></td><td></td><td></td></tr>
<tr><td>Büchner funnel</td><td>Hirsch funnel</td><td>Sintered glass funnel</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>356
357
364</td><td>The steps of recrystallisation to purify an impure solid include:
<table>
<tr><td>dissolving an impure solid gently in a minimum volume of a hot solvent</td><td>hot filtration of the resulting mixture to remove any insoluble impurities</td><td>cooling the filtrate slowly to allow crystals of the pure compound to form, leaving soluble impurities dissolved in the solvent</td><td>filtering, washing and drying the pure crystals</td></tr>
</table>

the solvent used for recrystallisation is chosen so that the compound being purified is completely soluble at high temperatures and only sparingly soluble at lower temperatures.
The solvent used should be:

<table>
<tr><td>immiscible with the liquid mixture or solution (usually water)</td><td>one in which the solute is more soluble in than the liquid mixture or solution (usually water)</td><td>volatile to allow the solute to be obtained by evaporation of the solvent unreactive with the solute</td><td>unreactive with the solute</td></tr>
</table></td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>358
359
362</td><td>Solvent extraction involves isolating a solute from a liquid mixture or solution by extraction using a different immiscible solvent in which the solute is also soluble.

the lower layer is run off into a container and the upper layer is poured into a second container and this process is repeated to maximise the quantity of solute extracted.
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
<tr><td>360
361</td><td>In solvent extraction, two immiscible solvents form two layers in the separating funnel.

solute dissolves in both solvents and an equilibrium establishes between the two layers.
the ratio of solute dissolved in each layer is determined by the equilibrium constant <i>K</i>
</td><td></td><td>☹</td><td>😐</td><td>☺</td></tr>
</table>

363	I know that the quantity of solute extracted is greater if a number of extractions using smaller volumes of solvent are carried out rather than a single extraction using a large volume of solvent.		☹	😐	☺
365a **366** **367**	The technique of melting point determination is important using melting point apparatus • the melting point of a substance is the temperature range over which the solid first starts to melt, to when all of the solid has melted. • the identity of a pure compound can be confirmed by melting point analysis and a comparison of the experimentally determined melting point with a literature or known melting point value.		☹	😐	☺
368	The determination of the melting point of a compound can give an indication of the purity of a compound • the presence of impurities in the compound lowers the melting point and broadens its melting temperature range • this is caused by disruption in intermolecular bonding in the crystal lattice.		☹	😐	☺
365b **369**	The determination of a mixed melting point involves mixing a small quantity of the product mixed with some of the pure compound. • the melting point value and the range of the melting temperature can be used to determine if the product and the pure compound are the same substance.		☹	😐	☺
370 **371** **372**	Chromatography is used to separate the components present within a mixture • substances are separated due to differences in polarity or molecular size. Thin-layer chromatography (TLC) causes separation by the distribution between the stationary phase (solid) and the mobile phase (liquid).  • different compounds will have different solubilities and adsorption to the two phases between which they are to be partitioned. • TLC involves spotting the sample to be analysed near one end of a sheet of glass or plastic that is coated with a thin layer of an adsorbent. • Plate is placed on end in a covered jar containing a shallow layer of solvent. • solvent rises by capillary action up through the adsorbent and differential partitioning occurs between the components of the mixture • the more strongly a given component of a mixture is adsorbed onto the stationary phase, the less time it will spend in the mobile phase and the more slowly it will migrate up the plate.		☹	😐	☺
373 **374**	How far the compounds are carried on a TLC plate depends on • how soluble the compounds are in the chosen solvent • how well they adhere to the plate. • a developing agent or ultraviolet light is normally required to visualise the spots on a TLC chromatogram.		☹	😐	☺
375 **376**	I can calculate R_f values using: $R_f = \dfrac{\text{Distance travelled by the sample}}{\text{Distance travelled by the solvent}}$ • a compound always has the same R_f value (within experimental error) under the same conditions (temperature, solvent, and saturation levels)		☹	😐	☺
377	I know that the identity of a compound can be confirmed by: • comparing the experimentally determined R_f values with a literature or known value determined under the same conditions • making a direct comparison on a TLC plate between the compound being tested and the pure substance where a co-spot could be used		☹	😐	☺
378	TLC is used to assess the purity of substances • a pure substance should appear as a single spot (when spotted and developed on a TLC plate) • the presence of more than one spot shows that impurities are present. (although some impurities may not be visible by TLC analysis).		☹	😐	☺