

Core Topics

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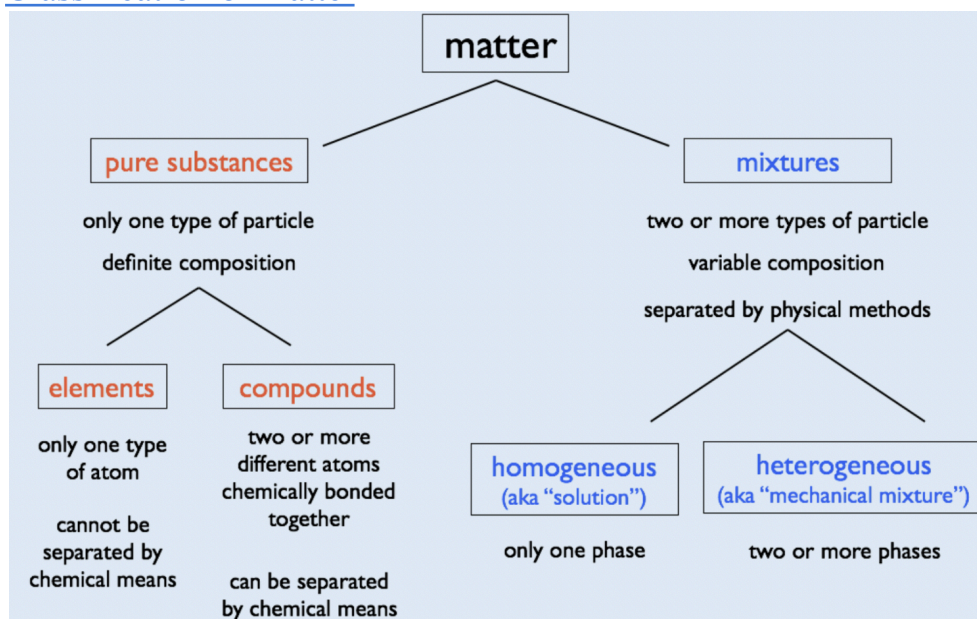
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Topic 1: Stoichiometric relationships

1.1 Introduction to the particulate nature of matter and chemical change

Classification of matter



Chemical vs physical change

- There is a change in the composition of a substance in a chemical change but not a physical change
- Examples of chemical changes: burning, rusting, cooking, rotting, acid-base reaction
- Examples of physical changes: freezing, melting, sublimating, evaporating, condensing, breaking a glass, spreading/stretching/bending a solid, dissolving

Chemical equations and types of reactions

- When a chemical equation is balanced, the number of atoms of each type of element on the reactant side equals the number of atoms of each type of element on the product side.
- Types of reactions:

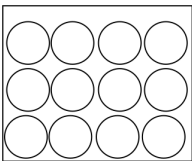
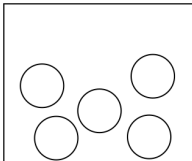
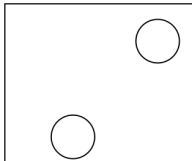
Reaction type	Description
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combustion	a fuel reacts with oxygen to release energy (exothermic reaction)
synthesis	two or more reactants combine to form a single product
decomposition	a complex molecule breaks down into simpler ones
single displacement	an element or group takes the place of another element or group in a compound
double displacement	ions switch places when two ionic compounds react

Kinetic Molecular Theory of Matter

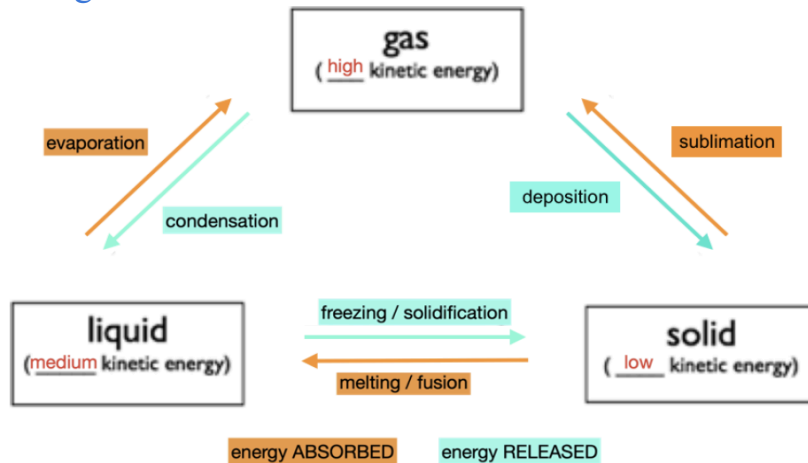
- 1) All matter is made of particles.
- 2) Particles are in constant, random motion.
- 3) The average kinetic energy of the system is directly proportional to its temperature, in Kelvin.
- 4) For ideal gases, there are no attractive forces between particles.
- 5) For ideal gases, the volume occupied by the gas particles themselves is negligible compared to the total volume occupied by the gas.
- 6) For ideal gases, collisions between gas particles are perfectly elastic (no energy is lost when they collided with each other or the walls of the container).

States of Matter

	solids	liquids	gases
arrangement and spacing of particles			
relative kinetic energy of each state	lowest	Intermediate	highest
types of motion*	vibrational	vibrational, rotational (very limited translational)	vibrational, rotational and translational
strength of forces of attraction between particles	strong	intermediate	weak
shape	definite / fixed	indefinite / not fixed	indefinite / not fixed

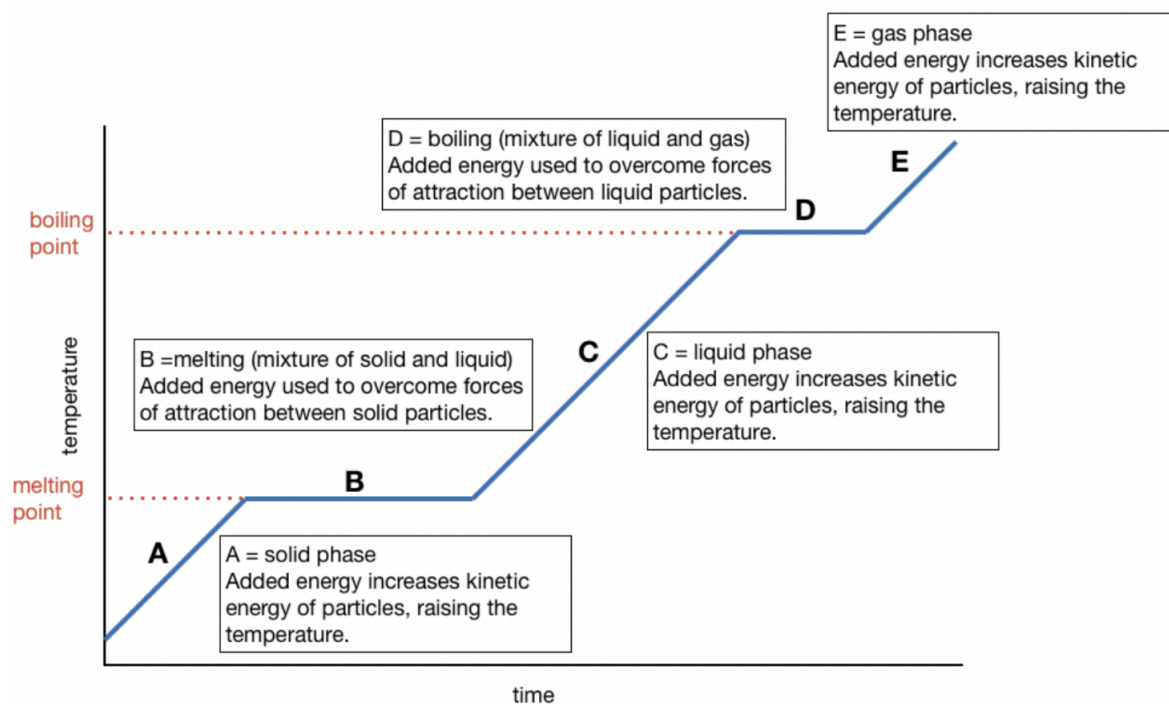
volume	definite / fixed	definite / fixed	indefinite / not fixed
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Changes of State



Heating and cooling curves

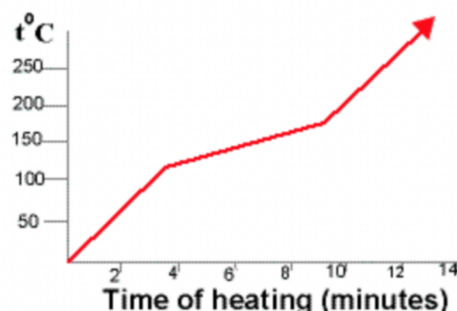
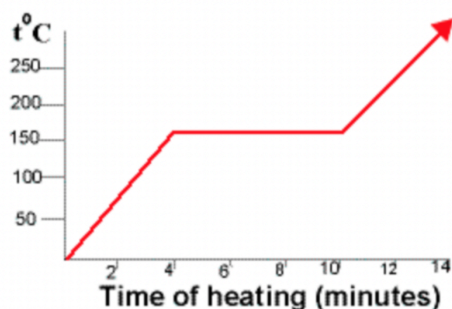
Heating curve for a pure substance:



- Cooling curves are similar, but reversed
- During the periods in which the temperature of the substance remains the same despite the substance being continuously heated, the added energy is being used to break the forces of attraction between the particles during the change of state.
- An impure substance will not have exactly straight horizontal lines during changes of state; instead of a singular temperature during changes of

state, there will be a range. In addition, the presence of a second type of particle in the mixture disrupts the regular arrangement of particles in the first substances. This weakens the intermolecular forces between the particles so less energy is required for melting/boiling.

Ex: Pure vs impure substance (pure on left, impure on right) heating curve



1.2 The mole concept

Introduction to the mole

- 1 mole is 6.02×10^{23} number of particles
- This value (6.02×10^{23}) is known as Avogadro's constant
 - 6.02×10^{23} is equivalent to the number of atoms in exactly 12g of carbon-12 atoms
- Avogadro's number: symbol = N_A (or L)
- Mole: symbol = n , unit name = mole, unit abbreviation = mol

Mass values

	symbol	meaning	units
relative atomic mass	A_r	the weighted average mass of an atom compared to 1/12 the mass of an atom of carbon-12	none
relative molecular mass	M_r	sum of the relative atomic masses of all the atoms in a molecule	none
relative formula mass	M_r	same as relative molecular mass, but used for ionic compounds	none
molar mass	M	mass in grams of one mole of a substance - calculated in the same way as relative molecular mass or formula mass but with different units	g mol^{-1}

		- can be found using experimental data	
--	--	--	--

Empirical and molecular formula (EF and MF)

- Empirical formula of a compounds is the simplest ratio of atoms in the molecule
 - Empirical formulae are found by experimentation. A compound is either synthesized or decomposed to find the mass of each element in the compound. The mass data is used to find the moles of each element present, and then the lowest mole ratio of each element.
- Molecular formula shows the actual number of atoms present in the molecule instead of just the ratios

Deriving MF from EF

Example: An organic carboxylic acid has the empirical formula CH_2O . Its relative molecular mass is 150.15. Determine its molecular formula.

$$\begin{aligned}\text{ratio} &= \frac{M_r(\text{actual})}{M_r(\text{EF})} \\ &= \frac{150.15}{30.03} \\ &= 5\end{aligned}$$

$$\begin{aligned}\text{MF} &= (\text{EF})_{\text{ratio}} \\ &= (\text{CH}_2\text{O})_5 \\ &= \text{C}_5\text{H}_{10}\text{O}_5\end{aligned}$$

Percentage composition by mass

There are two ways to find the percentage composition by mass of a compound:

1. Using the known chemical formula of the compound:

$$\% \text{ mass of element X} = \frac{\text{mass of X in the formula}}{\text{molar mass of the compound}} \times 100$$

2. Using experimental data (useful when the formula is not known):

$$\% \text{ mass of element X} = \frac{\text{mass of X in the sample}}{\text{total mass of the sample compound}} \times 100$$

Finding EF from percentage composition

Example:

Sulfur oxides, SO_x , are gaseous air pollutants. One sulfur oxide is 40.1% sulfur by mass and the rest is oxygen. Calculate the empirical formula of this gas.

1. Assume you have 100 g of the compound. Find the mass of each element in the compound.	$\text{mass S} = 100 \text{ g} \times 40.1/100 = 40.1 \text{ g}$ $\text{mass O} = 100 - 40.1 \text{ g} = 59.9 \text{ g}$
2. Find the amount, in moles, of each element.	$\text{mol S} = 40.1 \text{ g} \times \frac{1 \text{ mol}}{32.07 \text{ g}} = 1.25 \text{ mol}$ $\text{mol O} = 59.9 \text{ g} \times \frac{1 \text{ mol}}{16.00 \text{ g}} = 3.74 \text{ mol}$ Do not round off yet!
3. Find the lowest whole number mole ratio of each element by dividing all values by the lowest number of moles.	$\text{S: } \frac{1.25}{1.25} = 1$ $\text{O: } \frac{3.74}{1.25} = 2.99 \sim 3$ Whole number ratios are obtained so you can write the empirical formula.
4. Write the empirical formula.	EF = SO_3

Finding EF from combustion analysis

Example: A 0.5438 g of an unknown compound containing only carbon, hydrogen and oxygen was burned completely in oxygen. The products were 1.0390 g CO₂ and 0.6369 g H₂O.

1. Convert the mass of CO ₂ and H ₂ O to moles.	$\text{mol CO}_2 = 1.0390 \text{ g} \times \frac{1 \text{ mol}}{44.01 \text{ g}}$ $= 0.023601 \text{ mol}$ $\text{mol H}_2\text{O} = 0.6369 \text{ g} \times \frac{1 \text{ mol}}{18.02 \text{ g}}$ $= 0.03532 \text{ mol}$												
2. Convert the moles of CO ₂ to moles of C atoms in the unknown. <i>There is a 1:1 ratio of moles of C in the unknown to moles of CO₂ produced.</i>	$\text{mol C} = \text{mol CO}_2$ $= 0.023601 \text{ mol}$												
3. Convert the moles of H ₂ O to moles of H atoms in the unknown. <i>There is a 2:1 ratio of moles of H in the unknown to moles of H₂O produced.</i>	$\text{mol H} = \text{mol H}_2\text{O} \times 2$ $= 2 \times 0.03532$ $= 0.07068 \text{ mol}$												
4. Find the moles of O in the unknown. a) Convert moles of C and H in the unknown to mass. b) Find the mass of O in the unknown. c) Convert the mass of O to moles.	a) $\text{mass C} = 0.02361 \text{ mol} \times \frac{12.01 \text{ g}}{1 \text{ mol}} = 0.2836 \text{ g}$ $\text{mass H} = 0.07068 \text{ mol} \times \frac{1.01 \text{ g}}{1 \text{ mol}} = 0.07139 \text{ g}$ b) $\text{mass O} = 0.5438 - (0.2836 + 0.07139) = 0.1888 \text{ g}$ c) $\text{mol O} = 0.1888 \text{ g} \times \frac{1 \text{ mol}}{16.00} = 0.01180 \text{ mol}$												
5. Find the lowest whole mole number ratio of each element by dividing all values by the lowest number of moles.	<table><tr><td>C:</td><td>H:</td><td>O:</td></tr><tr><td>$\frac{0.02361}{0.01180}$</td><td>$\frac{0.07068}{0.01180}$</td><td>$\frac{0.01180}{0.01180}$</td></tr><tr><td>= 2.001</td><td>= 5.999</td><td>= 1.000</td></tr><tr><td>= 2</td><td>= 6</td><td>= 1</td></tr></table> ∴ the empirical formula is C₂H₆O	C:	H:	O:	$\frac{0.02361}{0.01180}$	$\frac{0.07068}{0.01180}$	$\frac{0.01180}{0.01180}$	= 2.001	= 5.999	= 1.000	= 2	= 6	= 1
C:	H:	O:											
$\frac{0.02361}{0.01180}$	$\frac{0.07068}{0.01180}$	$\frac{0.01180}{0.01180}$											
= 2.001	= 5.999	= 1.000											
= 2	= 6	= 1											

1.3 Reacting masses and volumes

Limiting and excess reactants (LR and ER)

- A limiting reactant is a starting material that determines the maximum amount of product that can form. The amount, in moles, of a limiting reactant determines the theoretical yield, in moles, of product. Once the limiting reactant is used up, no more product can form. The limiting reactant is usually entirely consumed in a reaction.
- An excess reactant is not completely used up in a chemical reaction. Some of it will remain after the reaction is over. This “leftover reactant” is usually considered as wasted material.
- Take care to note which reactant is limiting and which is excess when solving stoichiometric equations, using the coefficients given in the chemical equation.
 - 1) Find the moles of each reactant first if not given.
 - 2) Divide the moles of each reactant by their respective co-efficients.
 - 3) The LR is the reactant with the lower ratio.

Theoretical yield and experimental yield

- Theoretical yield (TY) is the amount of product formed if the reaction “goes to completion”. The TY is always a calculated value based on stoichiometry
- Experimental yield (sometimes called actual yield) is the mass of a product that you produce (or recover) from a reaction performed in the laboratory
 - During an experiment, you may lose material during transfers from one reaction vessel to another, lose material during filtration, or not completely separate one product from other products or unused reactants. These factors will all make the experimental yield different from the theoretical yield – sometimes lower and sometimes higher.

Percentage yield:
$$\text{percentage yield} = \frac{\text{experimental yield}}{\text{theoretical yield}} \times 100$$

Molar concentration

$\text{molar concentration} = \frac{\text{moles of solute}}{\text{total volume of solution in dm}^3} \quad \text{OR} \quad C = \frac{n}{V}$ concentration (C) units = mol dm⁻³ (sometimes abbreviated as M) n = mol volume (V) units = dm³

- A standard solution is one with known (and precise) concentration

Other concentration units

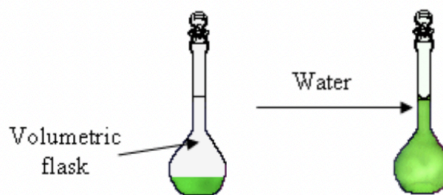
unit	meaning	example
% m/V	$\frac{\text{mass solute in g}}{100 \text{ cm}^3 \text{ solution}} \times 100$	0.8% saline solution (for intravenous drips) = 0.8 g NaCl / 100 cm ³
ppm (parts per million)	$ppm = \frac{mg \text{ solute}}{dm^3 \text{ solution}}$	25 ppm Pb ²⁺ = $\frac{25 \text{ mg Pb}^{2+}}{1 \text{ dm}^3}$

Preparing standard solutions

- A standard solution is a solution with a known and precise concentration.
- The preparation of a standard solution involves the use of a type of precision glassware known as a volumetric flask, which has very low measurement uncertainty and is known to be highly precise.
 - This type of glassware is used to prepare a defined volume of solution.
 - Water is added to the line on the neck of the flask to make a solution with a defined volume.

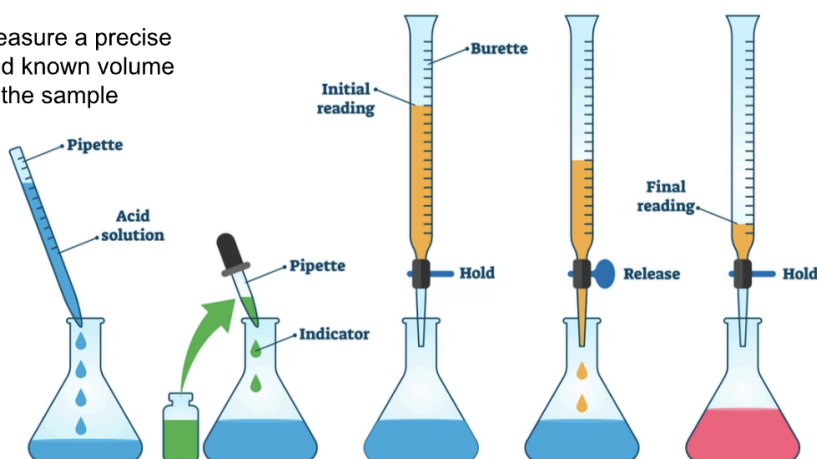
To prepare a standard solution, follow these steps:

- measure the mass of solid required
- transfer the solid to a beaker
- add a small volume of distilled water to the beaker (less than the desired final volume) and swirl to dissolve the solid
- once the solid is dissolved, transfer the solution to the volumetric flask
- add water to the flask up to the mark on the neck (with the bottom of the meniscus at the etched line on the neck of the flask)
- cap the flask and invert the flask several times to ensure complete mixing



Titration

measure a precise and known volume of the sample



- The solution in the burette- what you're using to try to find the concentration of the other solution- is the titrant. You know the precise concentration of this solution, both by calculations and also by titrating it against a primary standard.
- A primary standard is used to "standardize" another solution used in a titration. In other words, it is used to find the precise concentration of a solution.
- Some characteristics of primary standards are:
 - are available in very pure form
 - are stable in both solid and solution form
 - can dissolve easily in water
 - react completely in a known manner
 - have a relatively high molar mass
- The solution in the beaker- what you're trying to analyze- is known as the analyte

- You can use the below equation to identify concentrations of unknown solutions with a known volume using volumes of solutions with known concentration

Diluting solutions

- When we add water to a solution, or when we mix two solutions together, the concentration of the solute(s) is lower. This is called dilution.
- We may calculate the concentration of the solutes in the diluted solution or the mixture using this:

$$C_1V_1 = C_2V_2$$

C_1 = concentration of solute in original solution
mixture
(the most concentrated solution)
solution)

C_2 = concentration of solute in
(the less concentrated

V_1 = volume of original solution used
mixture ($V_1 + V_{H_2O}$)

V_2 = TOTAL volume of

Volume, Pressure and Temperature

The amount, in moles, of a gas in a chemical reaction can be measured experimentally in terms of a number of different quantities (e.g. mass or volume). Volume measurements in particular are dependent on the pressure and temperature conditions of the experiment in which a gas is used or produced.

quantity	meaning	units	unit equivalences
volume	amount of space occupied	cm^3 , dm^3 and m^3	$1 \text{ cm}^3 = 1 \text{ mL}$
		mL and L	$1 \text{ dm}^3 = 1 \text{ L} = 1000 \text{ cm}^3$ $1 \text{ L} = 1000 \text{ mL}$
pressure	force applied per unit area	Pa (Pascals) or kPa	$1 \text{ kPa} = 1000 \text{ Pa}$
		atm (atmospheres)	$1.00 \times 10^5 \text{ Pa} = 0.98692 \text{ atm}$
temperature	average kinetic energy of the particles in a substance	$^{\circ}\text{C}$ (degrees Celsius)	$^{\circ}\text{C} = \text{K} - 273$
		K (degrees Kelvin)	$\text{K} = ^{\circ}\text{C} + 273$

Standard Temperature and Pressure Conditions for Gases

STP (standard temperature and pressure)	T = 273 K P = 100 kPa = 1.00 x 10⁵ Pa
SATP (standard ambient temperature and pressure)	T = 298 K P = 100 kPa = 1.00 x 10⁵ Pa

Ideal vs Real Gases

An ideal gas displays these characteristics, at all temperatures and pressures:

- 1) Gases are made of very small particles separated by large distances. Most of the volume of a gas is empty space. The gas particles themselves occupy negligible volume.
- 2) Particles of a gas are in constant, random motion. They move in straight lines but random directions.
- 3) When particles of gases collide, the collisions are elastic. This means there is no energy lost in the collision.
- 4) There is no force of attraction between particles of the gas.

We assume that real gases behave in a similar way at high temperature and low pressure. However, they deviate most from ideal behaviour at low temperature and high pressure, particularly with respect to point 1 and point 4.



IDEAL GAS:
fast moving and widely spaced particles with almost no attractive forces



REAL GAS at LOW TEMPERATURES:
particles move more slowly so attractive forces are more important



REAL GAS at HIGH PRESSURES:
particles are packed closer together so the volume of gas particles is more significant and attractive forces are more important

Moles and Gas Volumes – Molar Volume at STP

Molar volume (V_{mol}) is the volume occupied by 1 mole of any gas at a certain temperature and pressure.

$$V_{\text{mol}} \text{ at STP} = 22.7 \text{ dm}^3 \text{ mol}^{-1} = 2.27 \times 10^{-2} \text{ m}^3 \text{ mol}^{-1}$$

Moles and Gas Volumes – Ideal Gas Law

The Ideal Gas Law relates pressure, volume, moles and temperature according to this equation:

$$PV = nRT$$

P = pressure in kPa

V = volume in dm³

n = amount in mol

T = temperature in K

R = gas constant = 8.31 J K⁻¹ mol⁻¹ (kPa dm³ K⁻¹ mol⁻¹)

Another form of the Ideal Gas Law replaces “n” with the mass (m) and molar mass (M) of the gas:

$$PV = \frac{m}{M}RT$$

The Law of Combining Volumes (LCV)

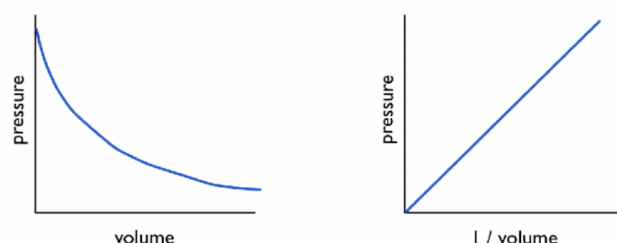
When gases react together to form other gases, and when all volumes are measured at the same temperature and pressure, the ratio between the volumes of reactant gases and products can be expressed in simple whole numbers.

- In other words, the volume ratio of the reacting gases is the same as the mole ratio in the balanced equation.
- Mole ratio = ratio of coefficients in the balanced equation

Boyle's Law

The pressure and volume of a gas are inversely proportional. As the pressure on a gas increases, its volume decreases. As the pressure on a gas decreases, its volume increases.

- Conditions: constant temperature and constant moles of gas

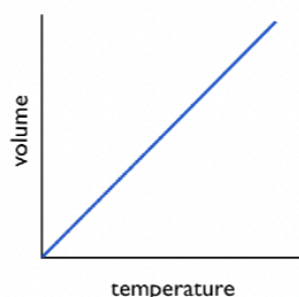
GRAPHICAL REPRESENTATION OF BOYLE'S LAW:**MATHEMATICAL EXPRESSION FOR BOYLE'S LAW:**

$$P_1 V_1 = P_2 V_2$$

Charles' Law

The volume and temperature of a gas are directly proportional. As the temperature of a gas increases, its volume increases. As the temperature of a gas decreases, its volume decreases.

- Conditions: constant pressure and constant moles of gas

GRAPHICAL REPRESENTATION OF CHARLES' LAW:**MATHEMATICAL EXPRESSION FOR CHARLES' LAW:**

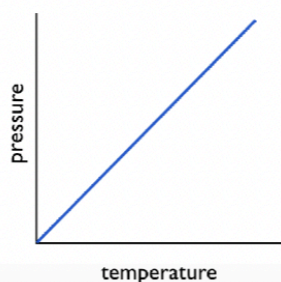
$$\frac{V_1}{T_1} = \frac{V_2}{T_2}$$

NOTE: Temperature must be in Kelvin.
(K = °C + 273)

Gay Lussac Law

The pressure and temperature of a gas are directly proportional. As the temperature of a gas increases, its pressure increases. As the temperature of a gas decreases, its pressure decreases.

- Conditions: constant volume and constant moles of gas

GRAPHICAL REPRESENTATION OF GAY-LUSSAC'S LAW:**MATHEMATICAL EXPRESSION FOR GAY-LUSSAC'S LAW:**

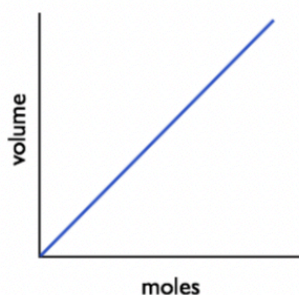
$$\frac{P_1}{T_1} = \frac{P_2}{T_2}$$

NOTE: Temperature must be in Kelvin.
(K = °C + 273)

Avogadro's Law

The volume of gas is directly proportional to the number of molecules (or moles), at constant pressure and temperature. As the number of moles of a gas increases, its volume increases. As the number of moles of a gas decreases, its volume decreases.

- Conditions: constant pressure and constant temperature

GRAPHICAL REPRESENTATION OF AVOGADRO'S LAW:**MATHEMATICAL EXPRESSION FOR AVOGADRO'S LAW:**

$$\frac{n_1}{V_1} = \frac{n_2}{V_2}$$

Combined Gas Law

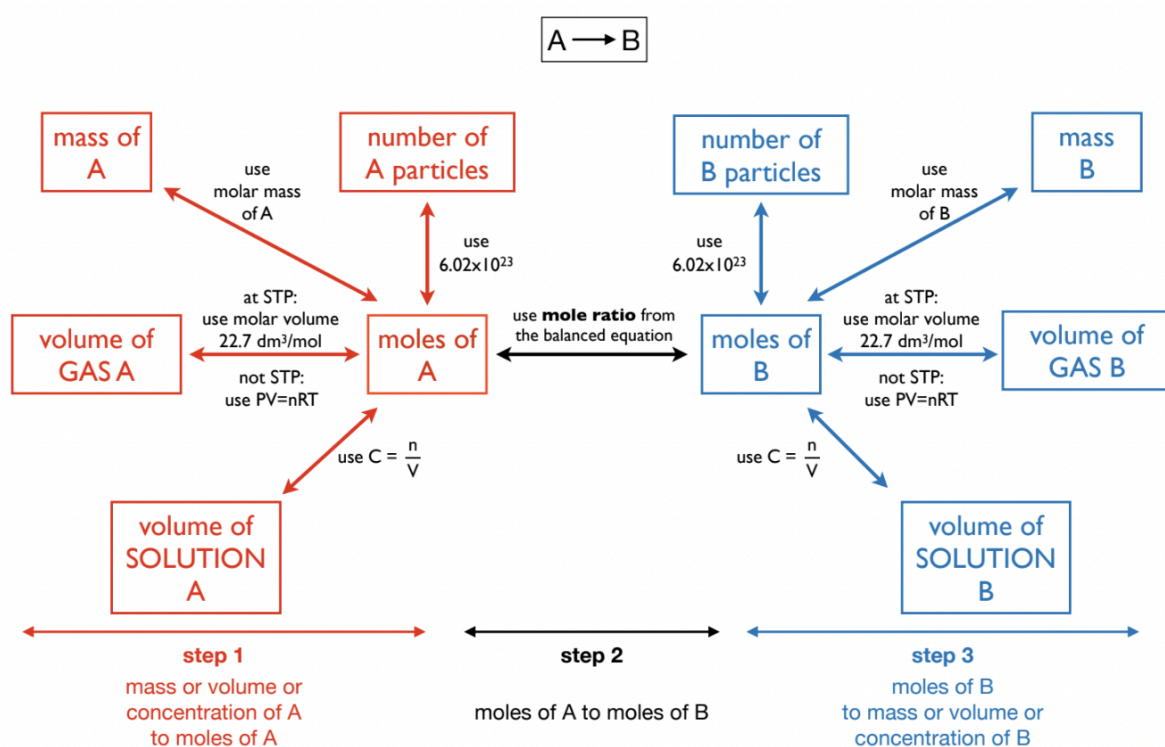
This is extremely useful for exams!

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

condition = constant amount, in moles, of gas

Stoichiometry Roadmap for calculations

Useful for exams!



Key terms for Topic 1

Term	Definition
Pure substances	substances with only one type of particle
Elements	substances with only one type of atom
Compounds	two or more different atoms chemically bonded together
Mixtures	two or more types of particle, and can be separated by physical means
Homogenous	mixtures that look the same throughout (only one phase)

mixtures	
Heterogenous mixtures	mixtures that don't look the same throughout (two or more phases)
Chemical change	a change in the composition of a substance
Balanced chemical equation	the number of atoms of each type of element on the reactant side equals the number of atoms of each type of element on the product side
Avogadro's constant	1 mole, aka 6.02×10^{23} number of particles
Relative atomic mass	the weighted average mass of an atom compared to 1/12 the mass of an atom of carbon-12
Relative molecular mass	sum of the relative atomic masses of all the atoms in a molecule
Relative formula mass	same as relative molecular mass, but used for ionic compounds
Molar mass	mass in grams of one mole of a substance
Empirical formula	the simplest ratio of atoms in a molecule
Molecular formula	the actual number of atoms present in a molecule
Limiting reactant	a starting material that determines the maximum amount of product that can form, is all used up in reaction
Excess reactant	reactant that is not completely used up in a chemical reaction
Theoretical yield (TY)	the amount of product formed if the reaction "goes to completion"
Experimental yield	the mass of a product that you produce (or recover) from a reaction performed in the laboratory
Standard solution	a solution with a known and precise concentration
Analyte	solution you're trying to find the concentration of

Titrant	solution with known concentration that you're using to try and find the concentration of the analyte
Primary standard	solution used to "standardize" the titrant
Molar volume (V_{mol})	the volume occupied by 1 mole of any gas at a certain temperature and pressure
The Law of Combining Volumes (LCV)	when gases react together to form other gases, and when all volumes are measured at the same temperature and pressure, the ratio between the volumes of reactant gases and products can be expressed in simple whole numbers
Boyle's Law	the pressure and volume of a gas are inversely proportional
Charles' Law	the volume and temperature of a gas are directly proportional
Gay Lussac Law	the pressure and temperature of a gas are directly proportional
Avogadro's Law	the volume of gas is directly proportional to the number of molecules (or moles), at constant pressure and temperature

Topic 2: Atomic structure

2.1 The nuclear atom

Rutherford and the Nuclear Atom

Gold foil experiment:

- Positive alpha particles (helium nuclei) were fired at a very thin sheet of gold foil, only a few atoms thick
- According to the Thompson model (the previous atomic model), the atom is a solid sphere with electrons (e-) embedded in a diffuse positive mass. Positive alpha particles should pass straight through without deflection.
- However, some positive alpha particles did pass straight through, but many were deflected by various degrees.
- Rutherford thus concluded that there must be a concentration of positive charge in the atom. The idea of a nuclear atom was developed.

Subatomic particles

particle	location	relative charge	mass (kg)	mass (amu)
proton	nucleus	+1	1.6726×10^{-27}	1
neutron	nucleus	0	1.6749×10^{-27}	1
electron	energy levels	-1	9.109×10^{-31}	0

Terminology related to atomic structure

- Atomic number (Z) = the number of protons in an atom
- Mass number (A) = the number of protons plus neutrons in an atom
- Number of neutrons = mass number - atomic number
- Number of electrons:
 - For neutral atoms: # e = number of protons
 - For cations (+ ions): # e = number of protons - charge
 - For anions (- ions): # e = number of protons + charge

Isotopes

- Isotopes are atoms of the same element with different numbers of neutrons. Isotopes are atoms with the same atomic number but different mass numbers.
- Radioisotopes are isotopes that have “unstable” nuclei
 - Unstable nuclei emit “radiation” as they try to become stable.
 - The three types of radiation are alpha, beta and gamma
- Examples of radioisotopes:
 - 1) Carbon-14: used for radioactive dating
 - 2) Cobalt-60 : used for cancer radiation therapy (breast cancer)
 - 3) Iodine-131: used for medical diagnosis (thyroid cancer)
 - 4) Uranium-235: used for nuclear power

Relative atomic mass

- It is the weighted average of all the naturally occurring isotopes of an element relative to carbon-12
- Symbol: A_r
- Takes the % abundance of each component into account when calculating weight of atoms

Example 1: Natural chlorine contains approximately 75% ^{35}Cl and 25% ^{37}Cl . Calculate its relative atomic mass.

What do we need? $\text{mass of each isotope} = \text{mass number}$
 $\text{abundance of each isotope} = \text{given (75\% = 0.75)}$

Solution:

$$\begin{aligned} A_r &= (\text{mass isotope 1})(\text{abundance isotope 1}) + (\text{mass isotope 2})(\text{abundance isotope 2}) \\ &= (35)(0.75) + (37)(0.25) \\ &= 35.5 \end{aligned}$$

Example 2: Iridium is composed of ^{191}Ir and ^{193}Ir .
Calculate the abundance of each isotope.

$$A_r = (\text{mass isotope 1})(\text{abundance isotope 1}) + (\text{mass isotope 2})(\text{abundance isotope 2})$$

What do we need? $A_r = 192.22$ (from the Periodic Table)

Let x = abundance of ^{191}Ir . Therefore abundance of $^{193}\text{Ir} = 1-x$

Solution:

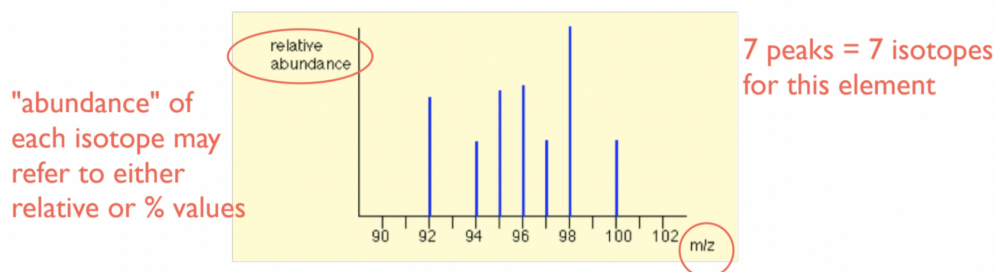
$$\begin{aligned} A_r &= (\text{mass isotope 1})(\text{abundance isotope 1}) + (\text{mass isotope 2})(\text{abundance isotope 2}) \\ 192.22 &= (191)x + (193)(1-x) \\ &= 191x + 193 - 193x \\ &= -2x + 193 \\ 2x &= 193 - 192.22 \\ x &= 0.39 \end{aligned}$$

Therefore the abundance of ^{191}Ir is 39% and that of ^{193}Ir is 61%.

Mass Spectrometer

- An analytic instrument used to measure the masses of the isotopes of an element and their abundances
- Can also be used to determine the composition of unknown molecular substances

A Mass Spectrum for an Unknown Element



m/z = mass/charge ratio

Most ions produced in the mass spectrometer have a charge of +1, so the m/z ratio is usually also the mass of each isotope.



Curious about how a mass spectrometer works? Watch this video. (This is not part of the DP Chem syllabus.)

2.2 Electron configuration

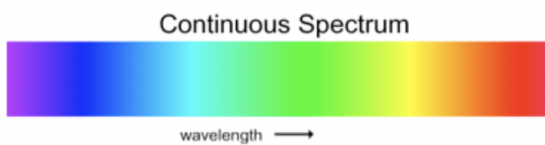
Discovery of atomic structure

- The Rutherford model asserted that:
 - the atom is mostly empty space
 - the nucleus is very small and positively charged

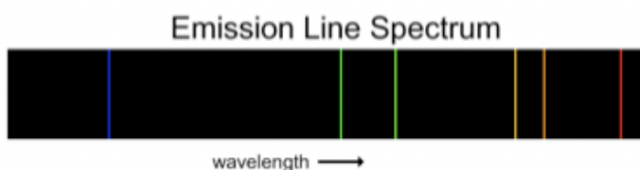
- electrons are found in the region around the nucleus
- However, the challenge presented by this is that according to the Rutherford model, there is nothing preventing electrons from spiralling straight into the nucleus
- To address the question of why electrons do not spiral into the nucleus, Niels Bohr proposed that the energy of electrons in an atom is quantized.
- This means that electrons are only allowed to have certain defined (or discrete) values of energy.
- Each energy level corresponds to a specific value of energy. Electrons are only found in an energy level with the same energy value as that of the electron. They do not spiral into the nucleus.
- Evidence for the Bohr model is provided by spectroscopes

Spectroscopes

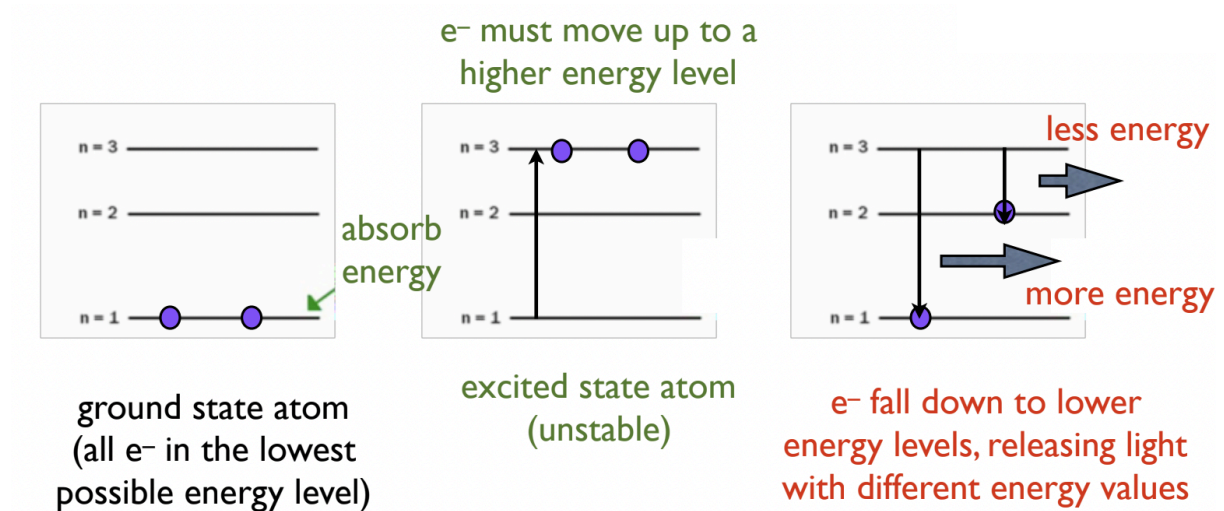
- A spectroscope is used to analyze the light emitted from a substance.
- It disperses incoming light into its component wavelengths.
- Two types of visible light spectra: continuous and dis-continuous
 - 1) Continuous: a light source that produces a continuous spectrum suggests that the source emits all energies of visible light.



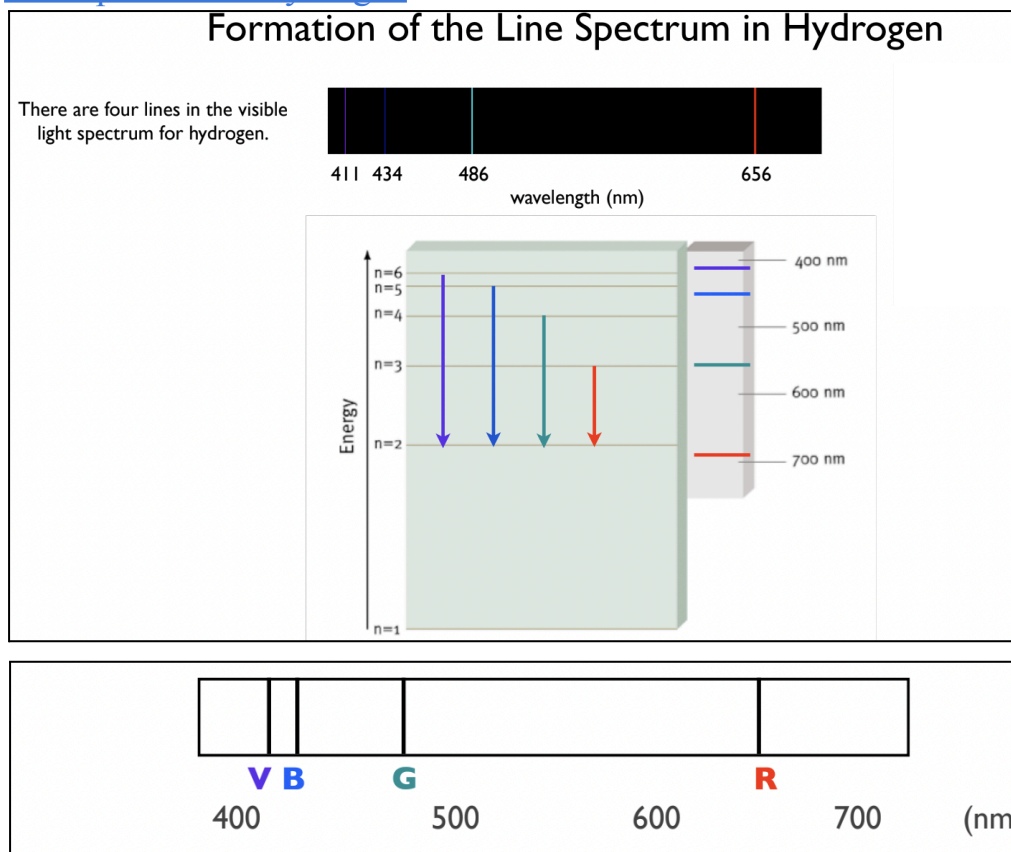
- 2) Non-continuous: A light source that produces a line spectrum (aka dis-continuous spectrum) suggests that the source emits only certain discrete energies of visible light.



- Process through which atoms emit light:

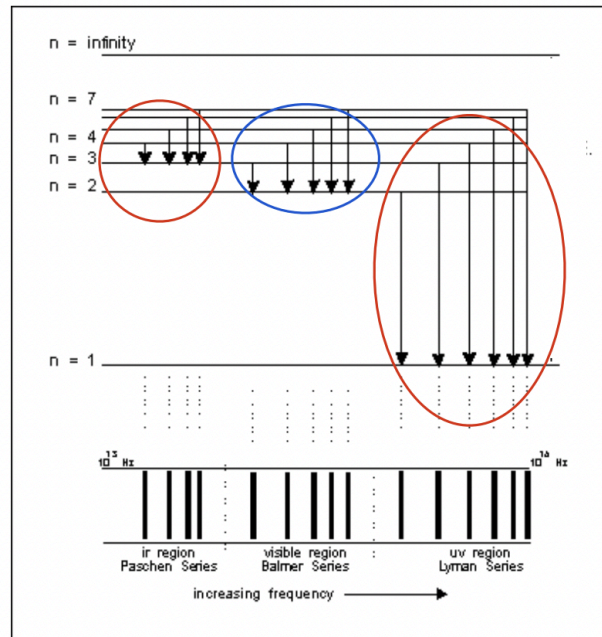


Line spectrum in hydrogen



- There are 3 series of atomic emission spectra in hydrogen:

Paschen series
infrared (lower E)
electrons fall to $n=3$



Balmer series
visible (intermediate E)
electrons fall to $n=2$

Lyman series
ultraviolet (higher E)
electrons fall to $n=1$

- The further the fall, the more the energy released

The quantum mechanical model

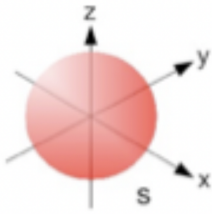
- The Bohr model held that:
 - electrons occupy defined energy levels
 - electrons are a fixed distance from the nucleus
 - electrons travel a predictable path
- The quantum mechanical model, a more recently developed one that we use to this day, holds that:
 - energy levels above $n=1$ have energy sublevels
 - within each sublevel, electrons occupy orbitals - regions of space with a high probability of finding an electron
 - orbitals do not have a fixed space
 - electrons move randomly within orbitals

Energy sublevels and orbitals

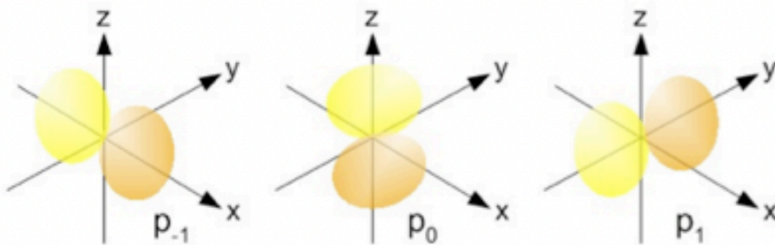
- Sublevels within an energy level have very similar energy values
- The number of sublevels in any energy level = n value
- The maximum number of electrons in each energy level = $2n^2$
- Sublevels are identified as s, p, d or f
- The energy of a sublevel slightly increases from $s \rightarrow p \rightarrow d \rightarrow f$

$n=1$	1 sublevel	1s
$n=2$	2 sublevels	2s 2p
$n=3$	3 sublevels	3s 3p 3d
$n=4$	4 sublevels	4s 4p 4d 4f

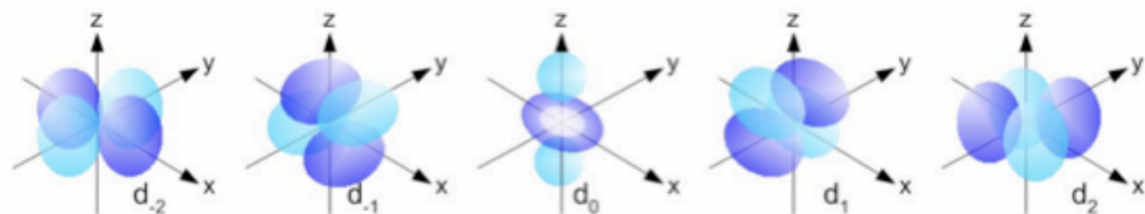
- An orbital is a region of high probability of finding an electron, and only holds 2 electrons
- Each type of sublevel contains a different number of orbitals and thus holds a different number of electrons
- The s sublevel has only one orbital (containing maximum 2 electrons), in a spherical shape



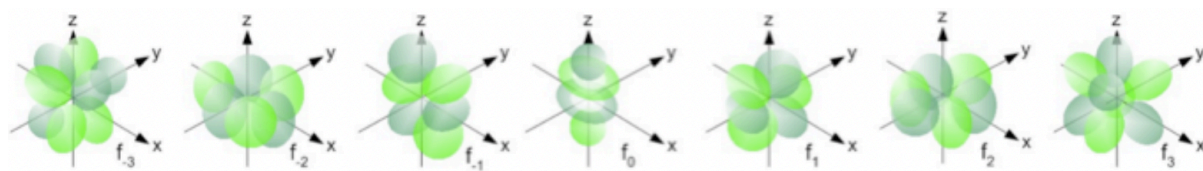
- The p sublevel has 3 “figure-8” shape orbitals (6 electrons maximum)



- The d sublevel has 5 orbitals with many orbital shapes such as cloverleaf or torus, and can contain 10 electrons maximum



- The f sublevel has 7 orbitals, many shapes, and can hold 14 electrons at max



- Each n has different sublevels

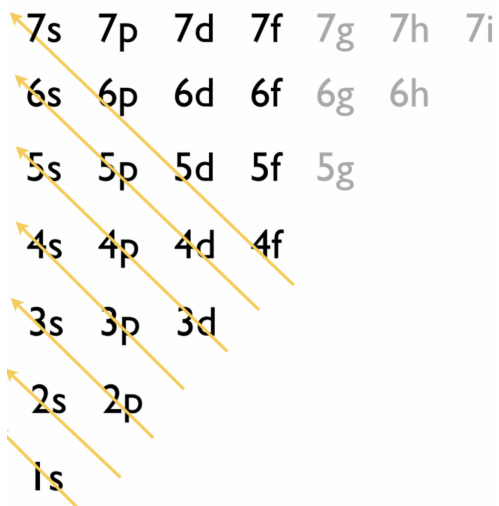
	$n=1$	$n=2$	$n=3$	$n=4$
# sublevels	1	2	3	4
types of sublevels	s	s, p	s, p, d	s, p, d, f
sublevel designation	1s	2s, 2p	3s, 3p, 3d	4s, 4p, 4d, 4f
# of orbitals	1	$1 + 3 = 4$	$1 + 3 + 5 = 9$	$1 + 3 + 5 + 7 = 16$
maximum # of electrons (2 e per orbital)	2	8	18	32

$$2n^2$$

Electron configuration rules

- Number of electrons per sublevel - Pauli Exclusion Principle
 - Each orbital has a maximum of 2 electrons
- Order of filling - Aufbau Principle
 - Electrons fill sublevels from the lowest energy level upwards. This gives the lowest possible potential energy for electrons in atoms.
 - The order of filling is more complicated after 3p is filled. The sublevels in higher energy levels start to overlap, as do their energy values
 - Exceptions are the transition metals. When there is $\text{__}s^2\text{__}d^4$, it will instead actually be $\text{__}s^1\text{__}d^5$, as then all the d orbitals will have an electron which is energetically favourable. Likewise, $\text{__}s^2\text{__}d^9$ will turn into $\text{__}s^1\text{__}d^{10}$, to fill all the d orbitals.

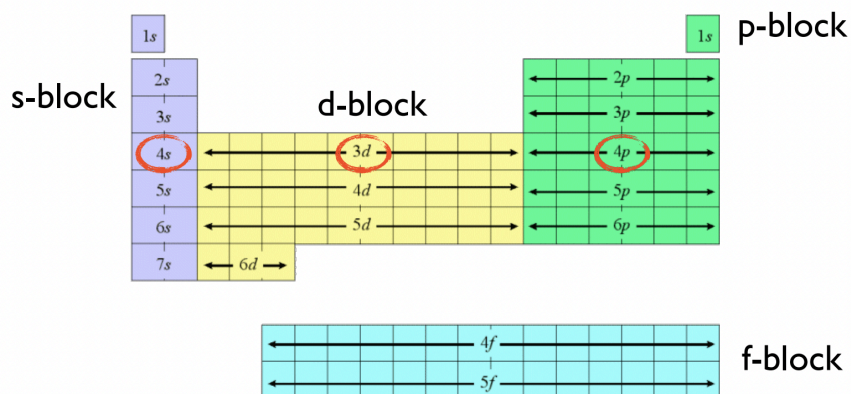
Order of filling:



Aufbau principle in the periodic table:

The Periodic Table follows the Aufbau order of filling as atomic number increases.

(Look at the electron configuration patterns at ptable.com)



- Hund's rule: Every orbital in a sublevel is singly occupied before any orbital is doubly occupied, and all of the electrons in singly occupied orbitals have the same spin (to maximize total spin).

Abbreviated electron configurations

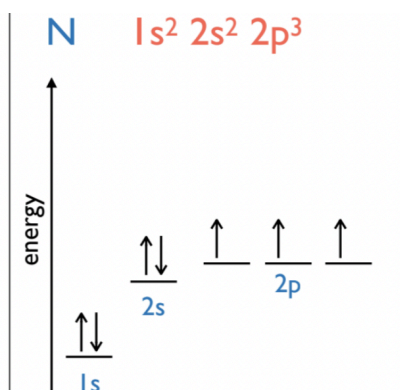
row 1	H	$1s^1$	
	He	$1s^2$	
row 2	Li	$1s^2 2s^1$	Li $[He] 2s^1$
	Be	$1s^2 2s^2$	
	B	$1s^2 2s^2 2p^1$	
	O	$1s^2 2s^2 2p^4$	O $[He] 2s^2 2p^4$
row 3	Ne	$1s^2 2s^2 2p^6$	
	Na	$1s^2 2s^2 2p^6 3s^1$	Na $[Ne] 3s^1$
	Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	
	P	$1s^2 2s^2 2p^6 3s^2 3p^3$	P $[Ne] 3s^2 3p^3$
row 4	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$	
	K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	K $[Ar] 4s^1$
	V	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$	V $[Ar] 4s^2 3d^3$
	Se	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^4$	Se $[Ar] 4s^2 3d^{10} 4p^4$
	Kr	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$	

- You can write the electron configuration of an element using: [symbol of noble gas before the element] + new electron configurations “added on-top” of the noble gas

Orbital box diagrams

- Orbital box diagrams are another way of showing how electrons are arranged in an atom.
- They give more information about the distribution of electrons in the orbitals in a given sublevel.
- Hund’s rule is relevant in orbital box diagrams, as electrons in the same orbital must be drawn with different spins. This can be done with one arrow (representing one electron) being drawn facing up and the other (representing the 2nd electron in the orbital) being drawn facing down. It is also important to remember that each orbital gets one electron each first before the electrons “double up” in an orbital, due to electron-electron repulsion.
- Orbital box diagrams may be drawn to show the relative energy of the different sublevels, with higher energy sublevels being further up

Example: Nitrogen



Key terms for Topic 2

Term	Definition
Atomic number (Z)	the number of protons in an atom
Mass number (A)	the number of protons plus neutrons in an atom
Number of neutrons	mass number - atomic number
Isotopes	atoms of the same element with different numbers of neutrons. Isotopes are atoms with the same atomic number but different mass numbers
Radioisotopes	isotopes that have “unstable” nuclei
Relative atomic mass	the weighted average of all the naturally occurring isotopes of an element relative to carbon-12
Mass spectrometer	an analytic instrument used to measure the masses of the isotopes of an element and their abundances
Spectroscope	instrument used to analyze the light emitted from a substance
Orbital	a region of high probability of finding an electron. Only holds 2 electrons
Pauli Exclusion Principle	each orbital has a maximum of 2 electrons
Aufbau Principle	electrons fill sublevels from the lowest energy level

	upwards. This gives the lowest possible potential energy for electrons in atoms
Hund's rule	every orbital in a sublevel is singly occupied before any orbital is doubly occupied, and all of the electrons in singly occupied orbitals have the same spin (to maximize total spin)
Orbital box diagrams	another way of showing how electrons are arranged in an atom. They give more information about the distribution of electrons in the orbitals in a given sublevel

Topic 3: Periodicity

3.1 Periodic table

Introduction to the Periodic Table

Periodic table of the elements

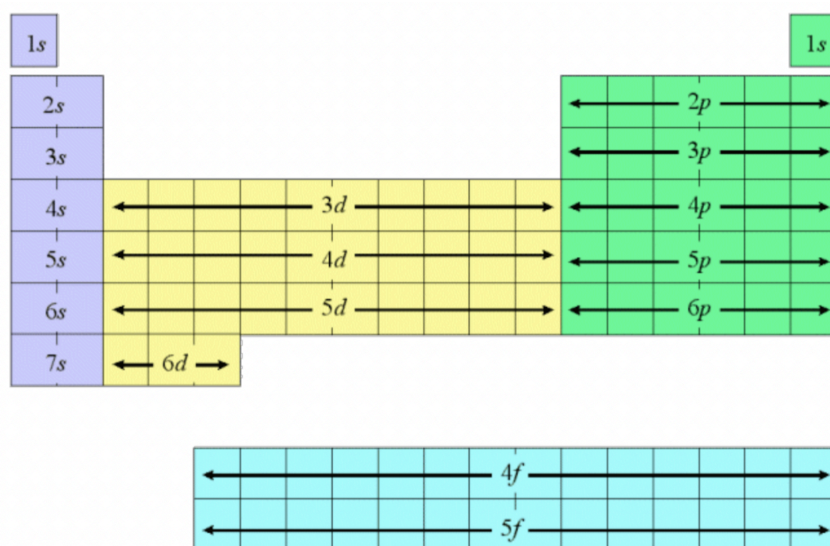
period	group	1*	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1		H																	He
2		Li	Be											B	C	N	O	F	Ne
3		Na	Mg											Al	Si	P	S	Cl	Ar
4		K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5		Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6		Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7		Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og
	lanthanoid series	6	58	59	60	61	62	63	64	65	66	67	68	69	70	71			
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Lu				
	actinoid series	7	90	91	92	93	94	95	96	97	98	99	100	101	102	103			
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

- Each column is a group and each row is a period
 - The period indicates the number of principal energy levels that the atom has
 - The period number (n) is the outermost energy level that is occupied by electrons (valence electrons)
 - The group indicates the number of valence electrons (more details below)
- Group 1 is alkali metals (highly reactive elements), each having one valence electron
 - Valence electrons are the electrons on the outermost shell (orbital) of atoms
- Group 2 is alkaline earth metals, each having two valence electrons
- Group 3-12 is transition metals. They can have many differing oxidation states.
- Groups 13-16 are metalloids and non-metals; metalloids fall under the staggered stair-step in the periodic table, and non-metals are above it. Group 13 has 3 valence electrons, 14 has 4, 15 has 5, and 16 has 6.
- Group 17 are halogens, highly reactive non-metals. They have 7 valence electrons each. They are one electron short of having the full outer s and p sublevel, which makes them very reactive.

- The halogens you need to memorize are: fluorine, chlorine, bromine, and iodine.
 - F_2 = gas, pale yellow
 - Cl_2 = gas, pale-green
 - Br_2 = liquid, deep-red with red-brown vapour
 - I_2 = solid, grey with purple vapour
- The terms lathanoids and actinoids (as depicted in the diagram above) should be remembered for exams.

Sublevels

- The periodic table has 4 blocks associated with the sublevels s, p, d, f as shown in the diagram below:



- The electron configuration of an atom can thus be deduced from the position of the element on the periodic table

3.2 Periodic trends

Trends in properties

1) Atomic radius

- Decreases down period due to the increased effective nuclear charge
- Increases down a group since increased number of orbitals and energy levels

2) Ionic radii

- Decreases from atomic radius if it is a cation since less electrons (e-) means greater pull due to less e- repulsion

- Increases from atomic radius if the ion is negatively charged due to e⁻ repulsion

3) Ionisation energy

- Energy (E) required to remove 1 mole of electrons from 1 mole of atoms in a gaseous state
- Increases across a period due to increased nuclear charge and decreased atomic radius
- Decreases down a group due to increased atomic radius, leading to decreased attraction between electrons and nucleus

4) Electronegativity

- Attraction of atom for bonding electron pairs
- Increases along a period since increased nuclear charge, decreased atomic radius
- Decreases down a group since increased radius

5) Electron affinity

- EA_1 = energy released when one mole e⁻ is added to one mole of atoms in a gaseous state, is exothermic
- EA_1 increases across a period, as the valence shells get increasingly closer to full (more stable)
- EA_1 decreases down a group as there is weaker attraction due to radius increase
- EA_2 is endothermic due to electron repulsion

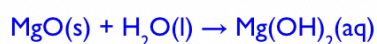
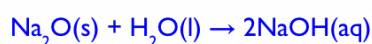
6) Metallic character

- Metallic character depends on the ability of an element to lose its outer valence electrons
- Metallic character increases down a group since the ionisation energy decreases going down a group and atomic radius increases going down a group
- Metallic character decreases going across a period

Acid/Base nature of Period 3 oxides

Na_2O	MgO	Al_2O_3	SiO_2	P_4O_{10}	SO_2 SO_3	Cl_2O Cl_2O_7
metal oxides (Group 1 + 2)			non-metal oxides			
basic		amphoteric	acidic			
$\text{pH} > 7$		variable pH	$\text{pH} < 7$			

metal oxide + H_2O
→ metal hydroxide



non-metal oxide + H_2O
→ oxyacid



Trends within groups

- Alkali metals are very soft, have low density, melting points (MP) and boiling points (BP) decrease down the group (metallic bonds, increased atomic radius leads to decreased strength of bonds - see Topic 4!), and alkali metals lose electrons easily
- Alkali metals undergo reactions with water to form metal hydroxide and $\text{H}_2(\text{g})$
- Reactivity of alkali metals increases down the group
- Halogen reactivity decreases down the group since there is less attraction
- Halogens get more solid further down the group since they have stronger IMFs in the form of London dispersion forces. The LDFs are stronger since the total number of electrons increases down the group.
 - For IMF content/elaboration, please see Topic 4.
- BP/MP of halogens increase down group since there is increased IMFs as stated above.

Key terms for Topic 3

Term	Definition
Atomic radius	the length of the radius of an atom
Ionic radii	the length of the radius of an ion

Ionisation energy	the energy required to remove 1 mole of electrons from 1 mole of atoms in a gaseous state
Electronegativity	a measurement of the attraction of an atom for electron pairs
Electron affinity	energy released when one mole of electrons is added to one mole atom in a gaseous state, is exothermic
Metallic character	the tendency of an atom to lose electrons and form cations (positive ions)

Topic 4: Chemical bonding and structure

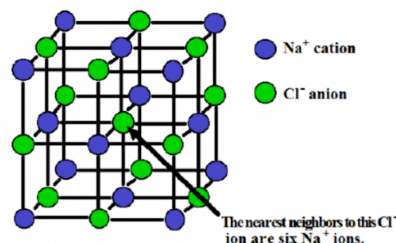
4.1 Ionic bonding and structure

Overview

- Ionic bonds are the electrostatic attraction between two oppositely charged ions
- A chemical bond is an electrostatic force of attraction that holds atoms together.
- Ions form when there is a transfer of electrons from one atom to another
 1. Valence electrons move from the atom with lower electronegativity (EN) to the atom with higher EN
 - EN = ability of atom to attract shared pair of electrons in a bond
 2. One atom becomes a cation, other becomes an anion
 - Cations are positive, anions are negative. Cations are formed from metals losing valence electrons, and anions are formed by non-metals gaining valence electrons.
 - The number of electrons gained or lost depends on the electron configuration of the atom:
 - Atoms in group 1 of the periodic table will have +1, group 2 = +2, group 13 = +3, group 14 = ±4, group 15 = -3, group 16 = -2, group 17 = -1
 - Noble gases don't form anions or cations due to their unreactive nature
 - Transition metals have variable oxidation states
 3. Electrostatic force of attraction holds the oppositely charged ions together in an ionic bond
- Ionic compounds form crystal lattice structures with cations and anions instead of forming individual molecules like covalent compounds
 - Lattice structure is very stable with ions in defined positions
 - Example: NaCl
 - Each cation is surrounded by 6 anions and each anion is surrounded by 6 cations

The lattice structure is a very **stable** structure.
Ions are in defined positions.

Example:
sodium chloride



Properties of ionic compounds

1. Brittleness
 - As force is applied to a crystal, one plane of ions shifts positions so that like charges are aligned
 - Strong repulsion between the like charges breaks the crystal
2. Electrical conductivity
 - Molten or aqueous ionic compounds have now-free-to-move ions (no longer trapped in lattice structure)
3. Volatility
 - Low volatility as force of electrostatic attraction strong so ions don't break free from solid/liquid to gas
 - Volatility = tendency of substance to vapourize
4. Solubility
 - High solubility in polar solvents
 - Hydration shell formed around ions due to the attraction between the charged particles and the dipoles of polar molecules, keeps the ions apart from each other so they cannot reelectrform the solid
 - Some cannot dissolve in polar solvents however because the the bond is too strong, cannot tear apart
 - Saturation = all H₂O used up in hydration shells, can't form any more
5. Melting point (MP) and boiling point (BP)
 - Have high MP and BP
 - Lots of E are needed to break bonds because the forces of attraction between cations and anions in a lattice structure are very strong
 - Increased charge = stronger attraction = more E needed to break bonds = higher MP/BP

Polyatomic ions

Element	Formula	Polyatomic name	Charge
—	OH	Hydroxide	1-
C	CN	Cyanide	1-
	HCO ₃	Bicarbonate	1-
	CO ₃	Carbonate	2-
N	NH ₄	Ammonium	1+
	NO ₂	Nitrite	1-
	NO ₃	Nitrate	1-
Cl	ClO	Hypochlorite	1-
	ClO ₂	Chlorite	1-
	ClO ₃	Chlorate	1-
	ClO ₄	Perchlorate	1-
S	SO ₃	Sulfite	2-
	SO ₄	Sulfate	2-
P	PO ₃	Phosphite	3-
	PO ₄	Phosphate	3-
Mg	MgO ₄	Permanganate	1-

4.2 Covalent bonding

Overview

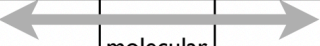
- A covalent bond is the simultaneous electrostatic attraction between a pair of electrons and positively charged nuclei
- Covalent bonds involve the sharing of electrons.
- More shared electrons = more bonds (eg double/triple bond instead of single) = bond strength increase = bond length decrease
 - Single bonds are longer and weaker than double bonds

- Bond enthalpy is the energy (E) required to break one mole of a given type of bond
- There are non-polar and polar covalent bonds (detailed below)
 - Bond polarity is a result of difference in electronegativity between the bonded atoms

Different types of covalent bonds

- Electronegativity (EN) is the measure of the tendency of an atom to attract a shared pair of electrons to itself
 - Elements higher in a group have higher EN
 - Metals have a lower EN than nonmetals
- Non-polar covalent bonds involve the equal sharing of electrons
 - $\Delta EN < 0.3$
 - ΔEN = difference in EN between the two atoms involved in the bond
- Polar covalent bonds involve unequal sharing of electrons, with the electrons shifting more towards one atom
 - $0.3 < \Delta EN < 1.7$
 - If $\Delta EN > 1.7$ then it is an ionic bond
- Dipoles are regions of partial charge. Negative dipoles form around atoms with higher EN, and positive dipoles form around atoms with lower EN in a bond.
 - Can use an arrow to represent bond dipole within a diagram, with the arrow head pointing towards the negative dipole.

Bonding in the Period 3 Oxides

formula	Na ₂ O	MgO	Al ₂ O ₃	SiO ₂	P ₄ O ₁₀ P ₄ O ₆	SO ₃ SO ₂	Cl ₂ O ₇ Cl ₂ O
ΔEN	2.5	2.1	1.8	1.5	1.2	0.8	0.2
bond type	Ionic	Ionic	Ionic	P. Cov	P. Cov	P. Cov	Cov
structure	 ionic			giant covalent	 molecular covalent		

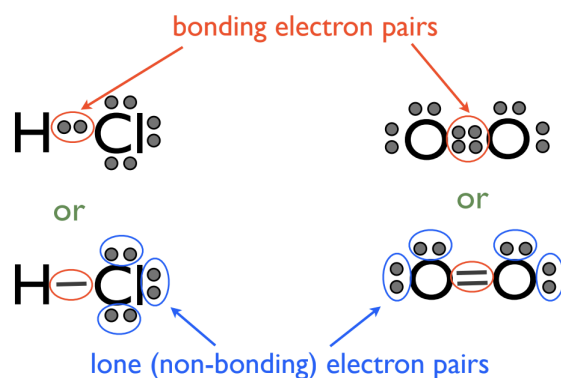
Bonding in the Period 3 Chlorides

formula	NaCl	MgCl ₂	AlCl ₃	SiCl ₄	PCl ₅ PCl ₃	S ₂ Cl ₂	Cl ₂
ΔEN	2.3	1.9	1.6	1.3	1.0	0.6	0.0
bond type	ionic	ionic	P. Cov	P. Cov	P. Cov	Cov	Cov
structure	←→ ionic		←→ molecular covalent				

4.3 Covalent structures

Lewis structures

Lewis structures (a.k.a electron dot diagrams) show the valence electrons of all atoms in a molecule as electron pairs.



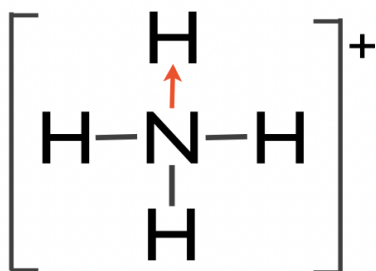
Drawing:

1. Count all valence electrons, adjust for ions
2. Write the element of the central atom, surrounded by that of the other atoms
3. Make covalent bonds by placing a bond in between the central atom and each other atom
4. Add pairs of electrons to the outer atoms, giving each a stable octet
 - This “octet rule” refers to the tendency of atoms to gain a “full” valence shell with a total of 8 valence electrons. However, there are a few atoms that can have incomplete octets, and also some that can have expanded octets.
5. Add any remaining pairs of electrons to central atom to create a stable octet, but if there are not enough electrons then make double/triple bonds
 - Some atoms can have incomplete octets (Be, B)

- Some atoms can have expanded octets due to unfilled d orbitals (eg $3s^2 3p^3 \rightarrow 3s^1 3p^3 3d^1$)
6. For polyatomic ions, place square brackets and charge around structure
 7. For multiple possible structures, use Formal Charge
 - Formal Charge = (number of valence electrons) - $\frac{1}{2}$ (number of bonding electrons) - (number of lone electrons)
 - $FC = \#VE - \frac{1}{2}\#BE - \#LE$
 - The structure with formal charge closest to 0 is preferred
 8. Sometimes the central atom in stable structures does not have an octet. Some atoms in Group 2 and 13, like Be and B, may form stable compounds with incomplete octets of electrons.

Coordinate covalent bonds

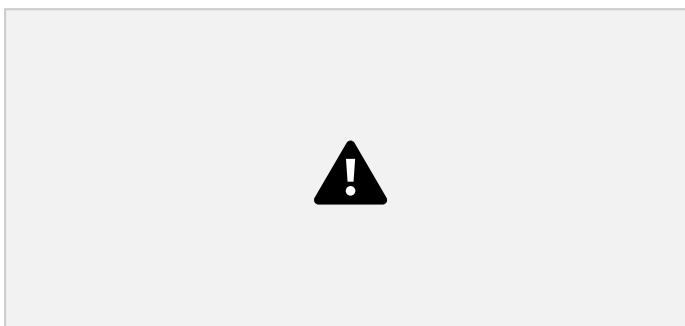
- Two electrons in the shared pair are provided by one atom
- An arrow symbol is used to represent coordinate covalent bonds, also called dative bonds, in Lewis structures- the arrow points towards atoms that receives electron pair
- Eg: NH_3^+ H_3O^+ CO



Delocalized electrons and resonance structures:

- Delocalization of electrons within a covalent molecule happens when there is more than one possible position for a double/triple bond within a molecule or a polyatomic ion
- Delocalization involves electrons that are shared by all atoms throughout the molecule, rather than localized between a pair of atoms
- With delocalized electrons, more than one Lewis structure is drawn, with a double-headed arrow in between them to indicate that the true structure is a blend of all the structures
- These structures are called resonance structures

Example: methanoate ion



- All the bonds in the structure with delocalized electron are the same bond length and bond energy, intermediate between double and single
 - Bond order is between double and single (1.5)
- For example in benzene, electron are delocalized and spread out evenly across all 6 C atoms

Properties of substances with delocalized electrons:

- 1) Intermediate bond lengths and bond strengths (as compared to single or double bond lengths between the same atoms)
- 2) Greater stability when electrons are delocalized, as electron-electron repulsion is less
 - Like repels like; electrons repel each other due to both having a negative charge

VSEPR Theory

- A theory that lets you predict the shape of small molecules!
- VSEPR = Valence Shell Electron Pair Repulsion
- The electron pairs in the valence shell will repel each other so that they are as far apart as possible.

- A VSEPR electron domain / electron pair can be:
 - 1) a lone (or non-bonding) electron pair (LEP)
 - 2) the one bonding electron pair (BEP) in a single bond
 - 3) the two bonding electron pairs (BEP) in a double bond
 - 4) the three bonding electron pairs (BEP) in a triple bond

Principles of VSEPR:

- Electron domains (EDs) around a central atom spread out as far apart as possible due to repulsion forces between electron pairs
- This minimizes the energy of the molecule (by minimizing the repulsive forces)
- Lone electron pairs have greater repulsive forces than bonding electron pairs
- Electrons in double bonds and triple bonds count as one electron domain

ED geometry, molecular geometry and bond angles of molecules depend on their number of EDs and number of LEPs.

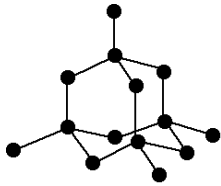
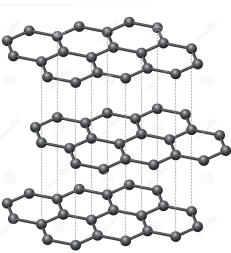
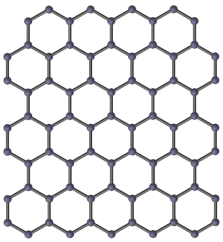
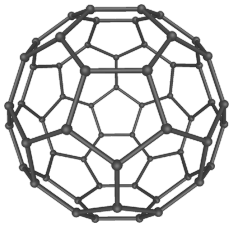
#ED	ED geometry	#LEP	Molecular geometry	Bond angle (°)
2	Linear	0	Linear	180
3	Trigonal planar	0	Trigonal planar	120
		1	Bent/angular	117
4	Tetrahedral	0	Tetrahedral	109.5
		1	Trigonal bipyramidal	107
		2	Bent/angular	104.5

Giant covalent and molecular covalent structures

- Carbon and silicon both form giant covalent structures.

Carbon allotropes

Name	Diamond	Graphite	Graphene	Fullerenes
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Diagram				
Structure	Made of C atoms covalently bonded to four other C atoms.	Made of C atoms covalently bonded to 3 other C atoms in hexagonal rings that form sheets. Sheets attach to each other due to LDFs.	A single sheet of graphite. C atoms are bonded to 3 other C atoms in hexagonal rings to form planar sheet 1 atom thick.	60 C particles in C ₆₀ fullerenes. C atoms are arranged in pentagonal and hexagonal shapes to form a sphere.
Molecular geometry, bond angles and hybridisation	Tetrahedral (109.5°) around each C atom, sp ³ hybridisation	Trigonal planar (120°), sp ²	Trigonal planar (120°), sp ²	Trigonal planar (120°), sp ²
Stability	Very stable structure, held together by strong covalent bonds and tetrahedral atom arrangement.	Within a sheet atoms are held together by covalent bonds, multiple sheets are held together by LDFs.	Sheet is held together by covalent bonds, so it is very stable.	Stable. C atoms are held together by covalent bonds.
Physical properties	Hardest known substance due to the stability of the structure.	Slippery, brittle, and can be used as machine lubricant because the London forces	Flexible, transparent, very strong, thin, highly conductive, stretchy, and impermeable.	NA

		between sheets are easily broken.		
Conductivity	Not conductive	Conductive because of delocalized electrons in the double C=C bond so electrons can move within a plane.	Conductive as delocalized electrons are present in C=C bond, making it possible for electrons to move within plane.	Poor conductivity as there are delocalized electrons within one molecule but they don't move to another molecule.

Silicon-based giant covalent structures

Name	Elemental silicon	Silicon dioxide
Structure	Giant covalent structure (like diamond)	SiO ₂ refers to the ratio of atoms inside the lattice structure. It is not made of SiO ₂ molecules.
Bonding	Si atom covalently bonded to 4 other Si atoms	Each Si atom is covalently bonded to 4 O atoms, and each O atom is covalently bonded to 2 Si atoms.
Molecular geometry, bond angles and hybridization	Tetrahedral, 109.5°, sp ³	Tetrahedral, 109.5°, sp ³
Conductivity	Semi-conductive	Non-conductive
Melting point (MP)	High MP	High MP

- In SiO₂, each silicon atom is central to a tetrahedron of four O atoms

4.4 Intermolecular forces

London dispersion forces (LDFs)

- Electrostatic force of attraction between all types of molecules
- Only type of force that holds non-polar molecules together
- Non-polar molecules don't have permanent dipoles because the electrons are equally distributed, but electrons are in constant random motion, so at any one time temporary dipoles may form
- Temporary dipole - temporary dipole
- When a molecule approaches another molecule, temporary dipoles may form and a weak electrostatic force of attraction holds molecules together; dipoles are constantly being formed and broken
- Strength of London forces depends on the number of electrons; more electrons = stronger since electron further from nucleus so polarizability of (larger) electron cloud greater

Dipole-dipole forces of attraction

- This is an electrostatic force of attraction between opposite dipoles on two molecules
- It forms between polar covalent molecules with permanent dipoles
- When molecules have the same number of electrons, presence of dipole-dipole forces increases the overall strength of IMFs within the molecule and thus increases the boiling point (BP), but when polar molecules have very different number of electrons or molar mass, the effect of London forces on strength of IMF is greater than the effect of dipole-dipole forces
- There are also induced dipole - dipole forces of attraction
 - Some polar molecules can induce a dipole on a non-polar molecule, which sets up an induced dipole - dipole force of attraction by distorting the electron cloud on the non-polar molecule
 - E.g. the polar H_2O molecule can induce a dipole on the non-polar O_2

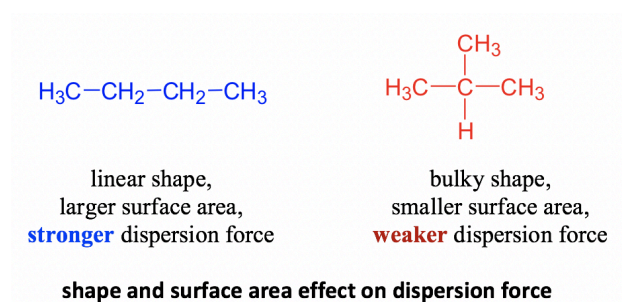
H bonds (hydrogen bonds)

- H bonds are a special case of dipole-dipole. They are the strongest IMF.
- They are an electrostatic force of attraction between the LEP on the strongly negative dipole on a F/O/N atom on one molecule and a strongly positive dipole on the H atom on another molecule

- More LEP = more H bonds = stronger IMF = increased BP

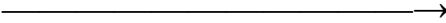
Inter-molecular forces (IMFs) in organic compounds (OCs)

- Two things affect the IMFs in OCs: functional groups and whether the OC is linear or branched
- The functional group determines what type of IMF the OC has
 - For example, if the functional group is hydroxyl the OC will have hydrogen bonding, but if it has no functional group (is an alkane), the OC will only have London dispersion forces.
- Linear vs branched:



For molecules in the same class, as length of R group increases the overall polarity of the molecule (net dipole moment) decreases, because there are more atoms that the electrons need to spread over

Summary table

Type of IMF	London forces	Dipole-induced dipole forces	Dipole-dipole forces	Hydrogen bonding
Relative strength				
Strength is dependent on	Number of electrons	Strength of dipole (for polar) + number of electrons (on non-polar)?	Strength of dipole	Number of LEP
What is needed	Unbonded electrons (for temporary dipoles)	1 dipole molecule + one not	2 molecules with permanent dipole	Strong positive dipole on H + strong negative

				dipole on F, O, N (need LEP)
Type of covalent molecule needed	non-polar	Mix of polar and non-polar	polar	Polar (with F, O, N + H)
Examples	I ₂	O ₂ and O ₃	HCl	H ₂ O

4.5 Metallic bonding

Overview

- Metallic bonds are the electrostatic attraction between metal cations and delocalized electron
 - Occur because metals have a low ionization energy and easily lose electron
 - Positively charged metal ions are left after metal atoms lose valence electron, when no non-metal electron are delocalized and are shared by all the metal cations, free to move within the metal
- Strength of bonds depends on cation charge and size
 - If the cation is larger in size, the distance between nucleus and valence electron is greater, so the force of attraction is weaker.
 - If the cation charge is greater, the force of attraction between nucleus and delocalized electron is greater and also there's more delocalized electrons, so the overall force of attraction is stronger.
 - Melting points of the metals reflects the strength of the metallic bonds.
- Metals have positive ions in fixed positions within a “sea of electrons”
 - Metal ions are fixed in a lattice structure, but electrons can move anywhere in the structure.

Properties of metals

- Metals are conductive because the delocalized electrons in the metal are free to move
 - However they are less conductive at higher temperatures because the ions vibrating reduces mobility of electrons.
- Metals are malleable (can be hammered into sheets) as the mobile electrons allow cations to slide around over each other

- Like ball bearings in oil
- Delocalized valence electrons prevent repulsion between the metal cations, so the atoms are able to slip past each other

Alloys

- Alloys are a mixture of two metals or a metal and a nonmetal
- Useful as
 1. Increase strength and hardness of metal
 2. Prevent corrosion/rusting
 3. Improve appearance of metal surface
- An alloy is harder and stronger than the two separate metals because the orderly arrangement of atoms is disrupted, reducing the ability of the layers of atoms from sliding over one another
 - Since the atoms sliding over each other are no longer the same size, it is harder for the atoms to slide about, hence making the mixture stronger and harder; thus alloys are stronger and harder than the pure metals by themselves.
- Because of the presence of non-directional bonds where an ion has the same attraction from all directions for delocalized electron, the alloy can still be held together by the strong electrostatic attractive forces between the cation and delocalized electrons

Key terms for Topic 4

Term	Definition
Chemical bond	an electrostatic force of attraction that holds atoms together
Ionic bond	the electrostatic attraction between two oppositely charged ions
Covalent bond	the simultaneous electrostatic attraction between a pair of electrons (electron) and positively charged nuclei
Electronegativity (EN)	the measure of the tendency of an atom to attract a shared pair of electron to itself
Dipoles	regions of partial charge
Coordinate	when two electrons in the shared pair are provided by one

covalent bonds (dative bonds)	atom
VSEPR theory	Valence Shell Electron Pair Repulsion theory
London dispersion forces (LDFs)	electrostatic force of attraction between all types of molecules. Type of IMF.
Dipole-dipole forces of attraction	an electrostatic force of attraction between opposite dipoles on two molecules. Type of IMF.
H bonds (hydrogen bonds)	special case of dipole-dipole where a H atom on one molecule is attracted to an F, O or N atom on another. It is the strongest IMF
Metallic bonds	the electrostatic attraction between metal cations and delocalized electrons
Alloys	a mixture of two metals or a metal and a nonmetal

Topic 5: Energetics/thermochemistry

5.1 Measuring energy changes

Energy and bonds

- All reactions use and release energy (E)
 - When bonds break, E is used
 - When bonds form, E is released as is now more energetically stable
- Energy is transferred between a system and its surroundings
 - System = chemicals in reaction (rxn)
 - Law of Conservation of Energy states that total E is conserved in rxns; $\Delta E_{\text{lost}} = \Delta E_{\text{absorbed}}$

Endothermic reactions

When the E used to break bonds in the reactants is greater than the E released, E is absorbed by system

- Energy used greater than energy released, hence the reaction absorbs E, with heat E taken from surroundings
- E absorbed overall
- Energy lost by surroundings, temperature of surroundings decreases

Exothermic reactions

When the E used is less than the E released so E released overall

- E released by system, E gained by surroundings
- Temperature of surroundings increases

Enthalpy

- “Heat content” of a substance
 - Temperature is a measurement of the average kinetic energy of particles
- Total “internal energy” of a substance, including PE (chemical bonds) and KE (motion)
- Symbol: H
- Units: kJ or J

Enthalpy change

$$\Delta H = H_{\text{products}} - H_{\text{reactants}}$$

- In endothermic reactions, E is absorbed so $+\Delta H$ (positive ΔH)
 - $H_{\text{products}} > H_{\text{reactants}}$
- In exothermic reactions, E is released so $-\Delta H$ (negative ΔH)
 - $H_{\text{products}} < H_{\text{reactants}}$

Thermochemical equations

- Add value of ΔH after the normal chemical equation
- Standard conditions = pressure is 100 kPa, molar conc is 1 mol dm⁻³, all substances in standard state (most stable state)

Heat, temperature and enthalpy

- Heat = a type of energy transfer that occurs as a result of temperature differences (there is more heat in a large ice bath than a small coffee)
- Temperature = a measure of the average kinetic energy of a substance
 - Does not depend on amount of substance
- Enthalpy = a measure of the total energy of a substance
 - Does depend on amount of substance
 - Sum of KE and PE (KE has 3 types; translational, rotational, vibrational)

Calculating heat change of a substance

$$q = (m) (c) (\Delta T)$$

- q = heat change (J or kJ)
- m = mass in grams
- c = specific heat capacity in Jg⁻¹K⁻¹ (spec heat cap is the energy required to raise the temperature of 1 g of a substance by 1K)
- $\Delta T = T_f - T_i$ (can be °C or K)
- Specific heat capacity of water = 4.18

Calorimetry

$$\Delta \text{heat}_{\text{system}} = -\Delta \text{heat}_{\text{surroundings}}$$

- Assumptions made in calorimetry:
 1. The heat released by the reaction is completely transferred to the water; there is no heat loss
 2. There is no heat transfer from the reaction to the reaction vessel, thermometer, surrounding air
 3. The specific heat capacity and density of the dilute solution is the same as water

Calculating enthalpy change using calorimetry

1. Find the heat change of water using $q = (m) (c) (\Delta T)$
2. Find the heat change (q) of reaction using $q_{\text{water}} = -q_{\text{reaction}}$
3. Find moles of limiting reactant (LR) in the reaction
4. Find ΔH using $\frac{\text{heat change of reaction in kJ}}{\text{moles of LR}} = \frac{x \text{ kJ}}{1 \text{ mol}}$, with ΔH (kJ) being x

Temperature corrections for slow reactions

- With slow reaction (rxns) comes heat loss

- Rate of cooling after rxn = rate of heat loss during rxn
- Using graph, extrapolate the line for rate of cooling after reaction backwards until you reach when the substance first started reacting
- Find T_{final} on the extrapolated line at the initial time when the reaction began
- This will allow you to determine T_{final} as though the rxn were instantaneous

Standard enthalpy of formation

- Energy change when 1 mole of a substance is formed from its elements in their standard states.
 - $\Delta H^{\circ}_{\text{formation}}$ for any element in standard state is 0
- 3 ways to find any $\Delta H_{\text{reaction}}$ using $\Delta H^{\circ}_{\text{formation}}$ values:
 - 1) Use Hess's Law (see section 5.2)
 - Get formation equations for all compounds in equation from Table 12
 - Manipulate formation equations to get target equation
 - 2) Draw an enthalpy cycle
 - 3) Use formula: $\Delta H_{\text{reaction}} = \Delta H^{\circ}_{\text{f (products)}} - \Delta H^{\circ}_{\text{f (reactants)}}$
 - This is from Hess's Law, seen below in section 5.2

Standard enthalpy of combustion

- The change in enthalpy produced when one mole of the substance is completely burnt in air or oxygen at standard conditions
 - Standard state refers to the normal, most pure stable state of a substance measured at 100 kPa and 298 K
 - Symbol for standard state is °
- 3 ways to find any $\Delta H_{\text{reaction}}$ using $\Delta H^{\circ}_{\text{combustion}}$ values
 - 1) Use Hess's Law (see section 5.2)
 - Get combustion equations for all compounds in equation from Table 12
 - Manipulate combustion equations to get target equation
 - 2) Draw an enthalpy cycle
 - 3) Use formula: $\Delta H^{\circ}_{\text{reaction}} = \Delta H^{\circ}_{\text{c (reactants)}} - \Delta H^{\circ}_{\text{c (products)}}$

5.2 Hess's Law

Hess's Law

Whenever a reaction may be expressed as a series of a number of small steps, then the enthalpy change of the reaction is the sum of the enthalpy changes of the small steps

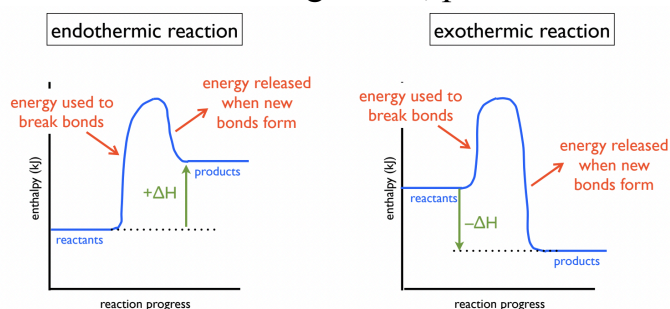
Algebraic calculations using Hess's Law

- 1) Manipulate the various equations you are given until get the equation you want
 - “Cancel out” the chemicals until the desired equation/reaction is reached
 - Equations may need to be flipped or multiplied by a certain factor
- 2) Change the enthalpy values as well according to how you manipulate the equations
 - Manipulating enthalpy values:
 - If an equation is written in reverse, ΔH needs to be multiplied by (-1)
 - If the coefficients of an equation are multiplied by factor (x) then ΔH also needs to be multiplied by (x)
- 3) Add the enthalpy values together to get the enthalpy value of the desired equation/reaction

5.3 Bond enthalpies

Bond enthalpy and average bond enthalpy

- Bond enthalpy = E required to break 1 mole of a given covalent bond in a molecule, under standard conditions. All reactants and products are in gaseous state.
- Average bond enthalpy = average energy used to break the bond in a range of different covalent molecules
- Forming a bond releases the same amount of E used to break the bond
- Forming bonds release energy, breaking bonds requires energy
 - In forming bonds, compounds become more stable
 - In breaking bonds, products are less stable than reactants



Estimating change in enthalpy using bond enthalpy

$$\Delta H = (\text{Sum of BE of reactants}) - (\text{Sum of BE of products})$$

Assuming:

1. Reactants and products are in gaseous state
2. Average of the bond enthalpy is the actual bond enthalpy in the molecules

Key terms for Topic 5

Term	Definition
Endothermic	when the energy (E) used to break bonds in the reactants is greater than the E released in product formation, resulting in temperature decrease of surroundings
Exothermic	when the E used is less than the E released, resulting in temperature increase of surrounding environment
Enthalpy	a measure of the total energy of a substance
Standard conditions	pressure is 100 kPa, molar concentration is 1 mol dm^{-3} , all substances in standard state (most stable state)
Heat	a type of energy transfer that occurs as a result of temperature differences
Temperature	a measure of the average kinetic energy of a substance
Standard enthalpy of formation	energy change when 1 mole of a substance is formed from its elements in their standard states
Standard enthalpy of combustion	the change in enthalpy produced when one mole of the substance is completely burnt in air or oxygen at standard conditions
Hess's Law	whenever a reaction may be expressed as a series of a number of small steps, then the enthalpy change of the reaction is the sum of the enthalpy changes of the small steps
Bond enthalpy	E required to break 1 mole of a given covalent bond in a molecule, under standard conditions. All reactants and products are in gaseous state.
Average bond enthalpy	average energy used to break the bond in a range of different covalent molecules

Topic 6: Chemical kinetics

6.1 Collision theory and rates of reaction

Chemical reaction rate

- Rate of a chemical reaction is defined as the change in the concentration of reactant or product per unit time
 - $\text{Rate} = \frac{\Delta[\text{reactant}] \text{ OR } \Delta[\text{product}]}{\text{time}}$
 - $[\text{x}]$ = concentration of x in mol dm^{-3}
 - Δ = change
 - Change in concentration = final value - initial value
 - Rate is usually in $\text{mol dm}^{-3} \text{ s}^{-1}$
 - This is for first-order reactions; HLs will learn about the orders of reactions, but SL will not
- Molar ratios can be used to calculate the rate of change for another substance when the concentration difference is not given in an exam question

Measuring reaction rate

Reactions	How to measure reaction rate
Any reaction	Rate can be measured by $\frac{\Delta[\text{reactant}] \text{ OR } \Delta[\text{product}]}{\text{time}}$
Reactions that produce gases	- Volume - Pressure - Total mass
Reactions with colour changes	- Absorbance - Will absorb light of complementary colour
Reactions with acids or bases	- pH
Reactions with concentration changes	- Conductivity
Chemiluminescent reactions	- Light intensity

- Can also measure by graphical analysis
 - Average rate of reaction = slope of line from start of reaction to point where reaction ends
 - Instantaneous = slope of tangent line at a given time

- Initial = slope of tangent (instantaneous rate) at $t=0$
 - Careful with choice of interval

Collision theory

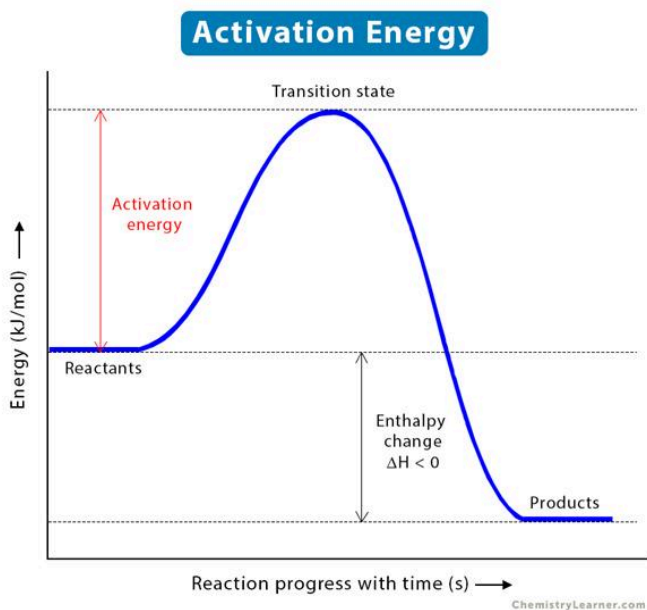
- Chemical reaction occurs only when reacting molecules collide successfully
 - Rate of reaction = frequency of success collisions

$$= \frac{\text{number of successful collisions}}{\text{time}}$$

$$= \frac{(\text{total number of collisions})(\text{fraction of successful collisions})}{\text{time}}$$
- For successful collisions:
 1. Reactants must collide with sufficient KE (kinetic energy)
 - Energy (E) needed to break reactant bonds and overcome electron repulsion
 - This minimum E needed to convert reactant to product is E_a , activation energy
 2. Must collide with correct geometry/orientation

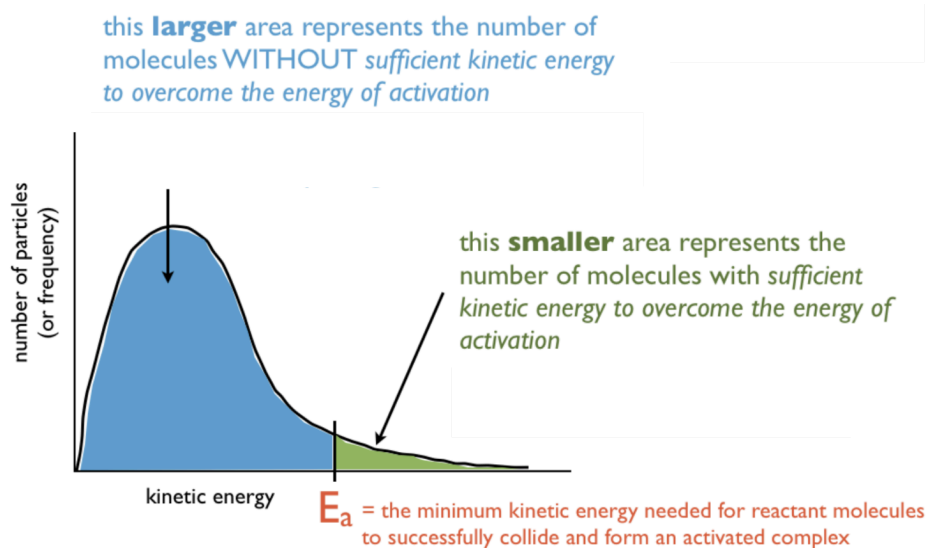
Activation energy

- Minimum E needed to convert reactant to product
- Reactants → activated complex (AC) aka transition state → products



- AC = high E, unstable transition state that forms when the reactants collide successfully
- Once the AC forms, reaction proceeds to form products
- Reactions with lower E_a value have a fast rate of reaction, reactions with higher E_a are slower
- E_a is equal to the difference in the potential energy of the reactants and the transition state.

Maxwell Boltzmann distributions



- Shows the number or frequency of molecules with a given KE
- Area under curve = total number of particles in sample
- High E_a = slow reaction, low E_a = fast
- The graph shows that, as the molar mass of the gas increases, the average molecular speed decreases. All of these gases have the same amount of kinetic energy.
- y-axis: number of particles, x-axis: KE

Factors affecting rate

1. Reactant concentration
 - Increased [reactant] = increased total number of collisions = more successful collisions per unit time = increased rate
 - Rate of reaction decreases over time throughout a reaction because the [reactant] decreases so fewer successful collisions occur per unit time
2. Pressure (for gaseous reactions only)
 - Pressure increases when volume decreases
 - Hence pressure increases when concentration increases
 - Increased pressure = greater number of total collisions
 - Particles further apart when reduce pressure, less collide
3. Surface area (SA)
 - High SA = small particle size = more total collisions
 - Low SA = big particle size = fewer successful collisions per unit time
4. Temp
 - Low temp = fewer molecules w/ sufficient KE to collide successfully
 - High temp = more molecules w/ sufficient KE = increased

frequency of successful collisions

- Temp changes affect:
 - a) Total number of collisions
 - b) Fraction of successful collisions
- A 10°C increase in temp will about double the rate of reaction

5. Catalyst

- Catalyst = chemical species which increases rate of reaction without being consumed in the reaction
- Provides alternate reaction mechanism with lower E_a
- Example: catalysis of hydrogen and oxygen using a heterogenous platinum catalyst
- A catalyst provides an alternative reaction pathway of lower activation energy for the forward and reverse reactions

Key terms for Topic 6

Term	Definition
Rate	$\frac{\Delta[\text{reactant}] \text{ OR } \Delta[\text{product}]}{\text{time}}$
Activation energy (E_a)	minimum E needed to convert reactant to product
Catalyst	chemical species which increases the rate of reaction without being consumed in the reaction. A catalyst provides an alternative reaction pathway of lower activation energy for the forward and reverse reactions.

Topic 7: Equilibrium

7.1 Equilibrium

Chemical equilibrium requirements

- 1) A reversible reaction
- 2) A closed system
 - Reactions with gases must be in sealed containers
 - Aqueous reactions can be in open containers

Chemical equilibrium characteristics

- 1) Rate of forward reaction = rate of reverse reaction
- 2) Macroscopic properties are constant; the reactant and product concentrations are constant but not necessarily equal
- 3) The system is dynamic; at the microscopic level, changes are still occurring
- 4) Equilibrium can be approached from either direction

Equilibrium Law

For $aA + bB \rightleftharpoons cC + dD$

$$K_c = \text{equilibrium constant} = \frac{[C]^c [D]^d}{[A]^a [B]^b} = \frac{[\text{reactants}]}{[\text{products}]}$$

- Remember that $[x]$ means the concentration of x, usually in mol dm^{-3}
- Solids are omitted from the K_c expression
- K_c values indicate what is favoured at equilibrium:
 - If $K_c = 1$ then neither reactants nor products are favoured at equilibrium
 - If $K_c < 1$ then reactants are favoured; the equilibrium lies to the left of the equation
 - If $K_c > 1$ then products are favoured; the equilibrium lies to the right of the equation

Manipulating chemical equations and K_c values

Change to equation	Effect on K_c
Reverse	$1/K_c$
Multiply coefficients by n	$(K_c)^n$
Divide coefficients by n	$(K_c)^{1/n}$
Add two equations together	$(K_1) * (K_2)$

Reaction quotient (Q)

- Q helps determine the progress of the reaction

$$Q = \frac{[C]^c[D]^d}{[A]^a[B]^b} \rightarrow \text{conc of reactants at ANY point in reaction}$$
- If $Q = K_c$ then reactants and products are at equilibrium, where the rate of the forward and the reverse reaction are the same
- If $Q < K_c$ then [reactant] greater and [product] lower than at equilibrium
 - Rate of forward reaction greater than reverse
 - Forward reaction favoured, reaction proceeds to the right
- If $Q > K_c$ then [product] greater and [reactant] lower than at equilibrium
 - Rate of reverse reaction greater than forward
 - Reverse reaction favoured, reaction proceeds to the left

Le Chatelier's Principle

If an equilibrium system is subjected to a stress, then the equilibrium responds in a way that reduces the effect of the stress and establishes a new equilibrium state.

- For example, if the concentration of A in $(A + B \rightarrow C + D)$ is increased, the equilibrium will shift to the right and the forward reaction (products) will be favoured

Effect of changing concentration on equilibrium

- If there is an increase in the concentration of reactants, [R], then the response to reduce stress will be to favour the products:
 - Forwards reaction favoured
 - Equilibrium shifts to right
 - There will be a rate change until equilibrium is restored; the forward reaction will be faster
- Other way around for if there is an increase in the concentration of product, [P]

Effect of changing temperature on equilibrium

- Heat should be treated like a product or reactant based on ΔH value given (whether the reaction is endothermic with $-\Delta H$ or exothermic with $+\Delta H$)
 - A change in temperature would thus result in similar outcomes to that detailed above in the "Effect of changing concentration on equilibrium" section
- For $-\Delta H$
 - Increase temperature = the system wants to "use up" heat by favouring the reverse reaction which is endothermic, so the equilibrium shifts to the left
 - Both forward and reverse reactions will go faster, but the reverse reaction will go faster than the forward reaction

- Decrease temperature = the system wants to produce more heat by favouring the forward reaction which is exothermic, so the equilibrium shifts to the right
 - Both forward and reverse reactions will be slowed, but the forward reaction will be faster than the reverse reaction
- It would be the other way around for $+\Delta H$
- Temperature is the only thing that affects K_c

Effect of changing pressure on equilibrium

- Pressure and volume are inversely related
- Increasing volume decreases pressure, making the system want to make more moles of gas, so the equilibrium shifts to the side with more moles of gas
- Decreasing volume increases pressure, so the reaction wants to make fewer moles of gas, so the equilibrium shifts to the side with fewer moles of gas

Effect of adding catalyst on equilibrium

- Increases the rate of both forward and reverse reactions equally so there is no shift in the equilibrium

Key terms for Topic 7

Term	Definition
Chemical equilibrium	the reactant and product concentrations in the reaction are constant, and the rate of the forward reaction is the same as the rate of the reverse reaction
Le Chatelier's Principle	if an equilibrium system is subjected to a stress, then the equilibrium responds in a way that reduces the effect of the stress and establishes a new equilibrium state
K_c (equilibrium constant)	$\frac{[\text{reactants}]}{[\text{products}]}$

Topic 8: Acids and bases

8.1 Theories of acids and bases

Theory 1: Bronsted-Lowry acid-base theory

- Acid = donates H^+
- Base = accepts H^+
- Conjugate pairs:
 - Acid / conjugate base = HA / A^-
 - Base / conjugate acid = B / BH^+
- Amphiprotic and amphoteric species
 - Amphiprotic = a species that can both donate and accept a proton
 - Amphoteric = acts as both acid and base (not necessarily amphiprotic)

Theory 2: Lewis acids and bases

- Lewis base = donates electrons
- Lewis acid = accepts electrons
- Nucleophiles (molecules drawn to areas of electron deficiency) act as Lewis bases by donating electrons
- Electrophiles (molecules drawn to electron-rich areas) act as Lewis acids by accepting electrons

8.2 Properties of acids and bases

Physical properties of acids and bases

- Taste - acids are sour, bases are bitter
- Feel - bases are slippery
- Strong acids and bases are very electrically conductive, weak ones are not

Chemical properties

- Metal + acid $\rightarrow$ salt + hydrogen gas
- Carbonate + acid $\rightarrow$ salt + water + carbon dioxide
- Metal hydroxide + acid $\rightarrow$ salt + water
- Base + acid $\rightarrow$ salt + water
- Metal oxide + acid $\rightarrow$ salt + water

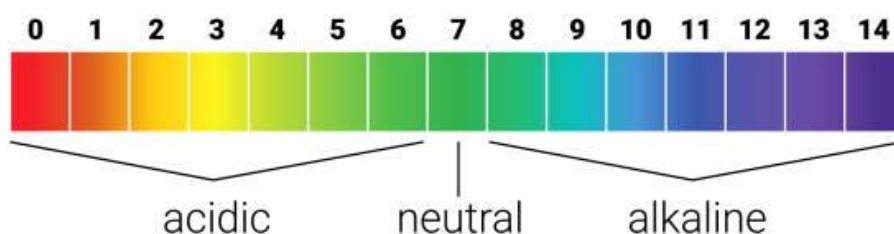
Salt and water are produced in exothermic neutralization reactions.

8.3 The pH scale

Overview

- pH is a measurement of the acidity of a solution; a measurement of the $[H^+]$ or $[H_3O^+]$ in a solution
 - $[H^+]$ means the concentration of H^+
- $pH = -\log_{10}[H_3O^+] = -\log_{10}[H^+]$
 - $[H_3O^+]$ and $[H^+]$ are interchangeable; both refer to proton (hydrogen ion) concentration
- $[H_3O^+] = 10^{-pH}$
- pH scale is logarithmic scale (as to represents larger numbers in a simpler way)
 - A one-unit change in pH is a ten-fold change in $[H^+]$
 - $[H^+]$ change = $10^{\text{change in pH}} = \text{change in "acidity"}$
- Acids have a pH of less than 7, bases have a pH of more than 7, and neutral solutions have a pH of around 7

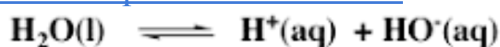
The pH scale



pH and pOH equations

- pOH is the same as pH except that it is for alkalinity instead of acidity
- $pH = -\log[H_3O^+] = -\log[H^+]$
 - One-unit change in pH is ten-fold change in $[H^+]$
- $[H_3O^+] = [H^+] = 10^{-pH}$
- $pOH = -\log[OH^-]$
- $[OH^-] = 10^{-pOH}$
- $pH + pOH = 14$

Water Equilibrium constant



- K_w = dissociation constant for water = $[H^+] * [OH^-]$
- At 25°C, $K_w = 1.00 * 10^{-14}$

- At any pH value, $[H^+] * [OH^-] = 1.00 * 10^{-14}$
 - $[H^+] = \frac{K_w}{[OH^-]} = \frac{1.00 \times 10^{-14}}{[OH^-]}$
 - $[OH^-] = \frac{K_w}{[H^+]} = \frac{1.00 \times 10^{-14}}{[H^+]}$

8.4 Strong and weak acids and bases

- Strong acids/bases completely dissociate
 - These reactions go to completion
 - If an acid is strong, it's conjugate base is weak
 - This is because strong acids completely dissociate, so the conjugate base has a low tendency of accepting H^+
 - "A strong acid like HCl donates its proton so readily that there is essentially no tendency for the conjugate base Cl^- to reaccept a proton. Consequently, Cl^- is a very weak base."
 - If a base is strong, it's conjugate acid is weak
 - This is because the conjugate acid has a low tendency of donating H^+
 - "A strong base like the H^- ion accepts a proton and holds it so firmly that there is no tendency for the conjugate acid H_2 to donate a proton."
- Weak acids/bases partially dissociate
 - These reactions are in equilibrium, with only some of the acid/base being ionized
 - For weak acids, the conjugate base has a strong tendency to accept H^+
- 6 strong acids: HCl, HI, HBr, H_2SO_4 , HNO_3 , $HClO_4$
 - Weak acids: carboxylic acids
- 4 strong bases: LiOH, NaOH, KOH, $Ba(OH)_2$
 - Weak bases: NH_3 , N_2H_4 , amines
- Strength does not equal to concentration; strength of acid/base is extent of dissociation, whereas concentration refers to amount of solute per unit volume
- Strong acids and bases are highly electrically conductive due to a high extent of dissociation; weak acids and bases are not

8.5 Acid deposition

Acid Rain

- Acid rain is defined as any rain with pH less than 5.6, usually 4-5
- Rain is naturally acidic as CO_2 dissolves in H_2O to create H_2CO_3 . However, carbonic acid is a weak acid and has a pH of 5.6
- Acid rain is created through sulfur oxide (SO_2) and nitrogen oxide (NO) emissions
- The acidic parts of acid rain are mainly the acids H_2SO_4 , H_2SO_3 , HNO_2 and HNO_3

Sulfur oxide formation

- Natural formation of SO_2 is when volcanoes explode
 - $\text{H}_2\text{S} + \text{O}_2 \rightarrow \text{SO}_2 + \text{H}_2\text{O}$
- Generation of SO_2 from man-made activity is from burning coal
 - $\text{S} + \text{O}_2 \rightarrow \text{SO}_2$
- SO_2 is a primary pollutant
 - A primary pollutant is an air pollutant emitted directly from a source. A secondary pollutant is not directly emitted, but forms when primary pollutants react in the atmosphere.

Sulfur oxide reactions

- 1) $2\text{SO}_2 + \text{O}_2 \rightarrow 2\text{SO}_3$
- 2) $\text{SO}_2 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_3$
- 3) $\text{SO}_3 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_4$

It is the acids H_2SO_3 and H_2SO_4 - particularly H_2SO_4 which is a strong acid - that makes acid rain so acidic.

Reducing SO_2 emissions - precombustion

- 1) Hydrosulfurization
 - Sulfur impurities are removed from fuel before combustion and turned into H_2S , using the CoMo catalyst, high pressure, and high temperature.
- 2) Use high grade of coal that has fewer sulfur impurities

Reducing SO_2 emissions - postcombustion

- 1) Spraying SO_2 gas with wet alkaline mixture
 - $\text{SO}_2 + \text{Mg}(\text{OH})_2 \rightarrow \text{MgSO}_3 + \text{H}_2\text{O}$
 - $\text{CaO} + \text{SO}_2 \rightarrow \text{CaSO}_3$
 - $\text{CaCO}_3 + \text{SO}_2 \rightarrow \text{CaSO}_3 + \text{CO}_2$
- 2) Fluidized limestone beds: mixing powder with the coal
 - $\text{CaO} + \text{SO}_2 \rightarrow \text{CaSO}_3$
 - $2\text{CaO} + 2\text{SO}_2 + \text{O}_2 \rightarrow 2\text{CaSO}_4$

NO formation

- NO naturally forms through lightning
- The anthropogenic (man-made) formation of NO is through vehicle emissions
 - $\text{N}_2 + \text{O}_2 \rightarrow 2\text{NO}$
- NO is a primary pollutant

NO reactions

- 1) $2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2$
- 2) $2\text{NO}_2 + \text{H}_2\text{O} \rightarrow \text{HNO}_2 + \text{HNO}_3$
- 3) $4\text{NO}_2 + \text{O}_2 + 2\text{H}_2\text{O} \rightarrow 4\text{HNO}_3$

The acids HNO_2 and especially HNO_3 (nitric acid is a strong acid) make acid rain acidic.

Reducing NO emissions

Using catalytic converters in car exhaust systems

- Pb, Pt, Rh catalysts
- $2\text{NO}_2 \rightarrow \text{N}_2 + 2\text{O}_2$

Effects of acid deposition (acid rain) on limestone

Calcium sulphate is more soluble in water than CaCO_3 . This leads to erosion of the limestone surface, as limestone is turned into calcium sulphate by acid rain, and the calcium sulphate is then washed away by water.

- 1) $\text{CaCO}_3 + \text{H}_2\text{SO}_4 \rightarrow \text{CaSO}_4 + \text{H}_2\text{CO}_3$
- 2) $2\text{CaCO}_3 + 2\text{SO}_2 + \text{O}_2 \rightarrow 2\text{CaSO}_4 + 2\text{CO}_2$
- 3) $\text{CaCO}_3 (\text{s}) + 2\text{HNO}_3 (\text{aq}) \rightarrow \text{Ca}(\text{NO}_3)_2 (\text{aq}) + \text{H}_2\text{O} (\text{l}) + \text{CO}_2 (\text{g})$

Effects of acid deposition on metals

Corrosion occurs when metals are touched by the components of acid rain.

- 1) $\text{Fe} + \text{H}_2\text{SO}_4 \rightarrow \text{FeSO}_4 + \text{H}_2$
- 2) $\text{Fe} + \text{SO}_2 + \text{O}_2 \rightarrow \text{FeSO}_4$

Key terms for Topic 8

Term	Definition
Acids	donates H^+ or accepts electrons depending on which theory is used

Bases	accepts H^+ or donates electrons depending on which theory is used
Amphiprotic	a species that can both donate and accept a proton
Amphoteric	acts as both acid and base (not necessarily amphiprotic)
pH	a measurement of the acidity of a solution; a measurement of the $[\text{H}^+]$ or $[\text{H}_3\text{O}^+]$ in a solution
Strength of acids/bases	extent of dissociation of the acid or the base
Acid rain	any rain with pH less than 5.6, usually 4-5

Topic 9: Redox processes

9.1 Oxidation and reduction

Redox reactions

- Redox reactions are reactions that involve a transfer of electrons from one reactant to another
- Redox reactions have an oxidation half-reaction and a reduction half-reaction
 - Electrons (e^-) always move from the oxidation to the reduction
- Write half-equations with electrons, balance out charges on both sides
 - If reduction, will have e^- on left side
 - If oxidation, will have e^- on right side
- Oxidising agent (OA) = reactant that is reduced
- Reducing agent (RA) = reactant that is oxidised
- Movement of charge

	Reduction reactions	Oxidation reactions
Change in electrons	↑	↓
Change in oxidation number	↓	↑
Change in O atoms	↓	↑
Change in H atoms	↑	↓

Oxidation state rules

- Pure elements have an oxidation state of zero
- Oxidation state = charge for monatomic ions
- H usually +1
 - In metal hydrides, will be -1
- O usually -2
 - In peroxides is -1
- Group 1 = +1 and Group 2 = +2
- Group 17 in a binary compound = -1
- Oxidation states of all atoms in compound all add up to overall charge on compound
- Remember to always put the sign before the number for oxidation states

IUPAC names for polyatomic ions

Name = stem of first element+ate + (oxidation # of first element)

Metal reactivity series

- When metals react they lose electrons, so metals with a low IE (ionization energy) are the most reactive
- The more reactive the metal is, the stronger it is as a reducing agent
- Reactivity series can be used to predict feasibility of single displacement reactions
 - More reactive (higher in series) will displace less reactive in compound in displacement reactions
 - New metal and metallic ion form

Halogen reactivity series

- Reactivity series follows order in PT from most reactive at top to least at bottom
- When halogens react they tend to gain electrons (e-)
 - Halogens that gain e- easily are the most reactive
- Reactive halogens are reduced, so OA
 - More reactive = stronger OA
- Can be used to predict reactions
 - More reactive (higher) will displace less reactive in compound in displacement reactions
 - New halogen and new halide ion form

Redox titrations

- Disproportionation reaction- This is a reaction in which the same element is oxidized and reduced at the same time
- OA and RA act as analyte or titrant
- Endpoint is visible change, equivalence point is when all moles of analyte have reacted with titrant
- Permanganate (VII) titrations
 - MnO_4^- used as titrant, is strong oxidising agent
 - Half-eq under acidic conditions:

$$\text{MnO}_4^- + 8\text{H}^+ + 5\text{e}^- \rightarrow \text{Mn}^{2+} + 4\text{H}_2\text{O}$$
 - Acts as self indicator; has purple colour, so when all moles of analyte have finished reacting and when add new will only stay as

the original titrant, colour of solution will be same as colour of the titrant and permanganate offers a purple colour so it will turn from colourless to purple

- Iodine-thiosulfate titration
 - $\text{S}_2\text{O}_3^{2-}$ is titrant, reduces I_2 under acidic conditions
 - Equation: $2\text{S}_2\text{O}_3^{2-} + \text{I}_2 \rightarrow 2\text{I}^- + \text{S}_4\text{O}_6^{2-}$
 - Starch indicator is used; in presence of I_2 forms a blue-black complex, in absence is colourless
 - This titration is used to measure concentration of analyte, at endpoint the solution turns from blue to colourless

Balancing equations

- Goals:
 1. Atoms
 - # of atoms of each element is same on reactant and product side of equation
 2. Electrons
 - # of e^- gained in reduction half cell = # e^- lost in oxidation half-cell
 3. Charge
 - Total charge on right side = total charge on left
- Half-equation approach
 1. Write two half-equations showing e^- , balance each one individually
 2. Multiply each half-reaction by a certain factor so the # e^- gained = # e^- lost
 3. Add the two together, electrons will cancel out in final equation
- Sk A O H E method (for half-equations)
 - Sk - write skeletal equation with product and reactant only
 - A - balance all atoms except O and H
 - O - add H_2O to the side that needs O
 - H - add H^+ to the side needing H
 - E - add e^- to the side that is more pos until they balance out
 - Remember to make the e^- balance when putting two half-equations together

9.2 Electrochemical cells

Single displacement reactions

- Exothermic
- If electrons are directly transferred at the point of contact, it wastes the energy from the exothermic reaction
- Instead of direct transfer, e⁻ can be moved from one substance to another via conducting materials in an external circuit
 - Since the flow of e⁻ through conductor generates electricity
 - This is the essence of **voltaic cells**

Operation of voltaic cells

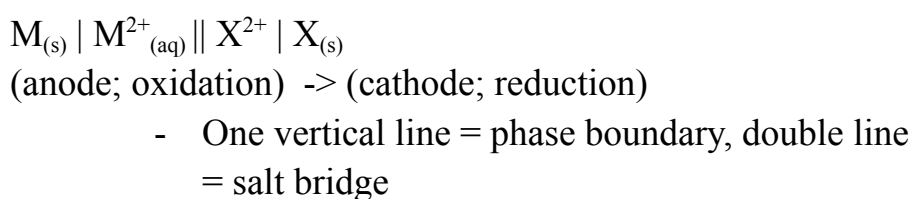
- Connecting wire between electrodes gives alternate path for electron movement between anode and cathode
- Components:
 1. Two half-cells
 - One oxidation one reduction
 - Cathode = reduction (positive electrode)
 - Anode = oxidation (negative electrode)
 - Each half cell has electrolyte (liquid) and electrode (conductor)
 2. Conducting wire/material between electrodes
 - Allows e⁻ to move from anode to cathode via external circuit (conductor)
 - Electrical current is generated
 - Transfers electrons from reducing agent (being oxidised) to oxidising agent (being reduced)
 3. Salt bridge between electrodes
 - Allows ions from the ionic solution in the salt bridge to move from the salt bridge to the half-cells, preventing the buildup of charge from the ion concentration increase/decrease (anion/cation) in the half-cells that would stop the reaction from proceeding because e⁻ movement would be impeded
 - Contains a solution of a soluble ionic compound (eg KNO₃)
- Role of salt bridge:

- In the oxidation half-cell (anode), the cation concentration builds up so anions from the salt bridge move to the anode to balance the charge
- In the reduction half-cell, the cations concentration decreases causing a buildup of negative charge, so the cations from the salt bridge move to the cathode to balance the charge and allow for unimpeded electron movement from the anode to the cathode
- Summary table for voltaic cells

	Anode	Cathode
Reaction	Oxidation	Reduction
Charge on electrode	Negative	Positive
Half equation	$M_{(s)} \rightarrow M^{2+}_{(aq)} + 2e^{-}$	$Y^{2+}_{(aq)} + 2e^{-} \rightarrow Y_{(s)}$
Change in electrode mass	Decrease	Increase
Salt bridge ion movement	Anion $\rightarrow$ anode	Cation $\rightarrow$ cathode
Electron flow	Anode $\rightarrow$ cathode (oxidation $\rightarrow$ reduction)	

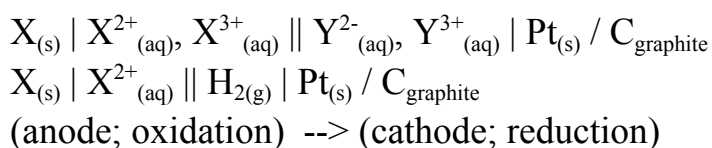
Cell diagram notation:

Normally:



Inert electrodes (see below also)

- Half-reactions occurring in some aqueous solutions may require inert electrodes which allow e^{-} to pass through without reacting
- Platinum or graphite (Pt or C)



Predicting reactions in voltaic cells

- The more reactive metal is oxidised to an ion, and ions of less reactive metal are reduced to solid
- Balance charge and combine both half-reactions for overall equation

Applications of electrolytic cells

1. Electrolysis of molten salts

- Extraction of metals/nonmetals from compounds in liquid form
 - Eg extracting pure metal from ores
- Elements can be purified by the electrolysis of *molten binary* salts (salt = electrolyte)
 - Has to be in liquid form, and binary means only 2 elements
- Done using inert electrodes
- Anode (positive electrode in electrolytic cells) = oxidation site where anions are oxidised
- Cathode (negative electrode) = reduction site where cations are reduced
- Overall equations
 - $\text{MY}_{2(l)} \rightarrow \text{M}_{(s)} + \text{Y}_{2(g)}$
 - $\text{M}^{2+} + 2\text{Y}^- \rightarrow \text{M}_{(s)} + \text{Y}_2$

2. Electroplating

- Application of a thin layer of a metal onto another object
- Electrolyte = aqueous ionic compound containing metal ion (M^{2+}) to be plated
- Anode = oxidation = source of plating metal M (replenishing M^{2+} in the solution)
 - $\text{M}_{(s)} \rightarrow \text{M}^{2+}_{(aq)} + 2\text{e}^-$
- Cathode = reduction = object to be plated
 - $\text{M}^{2+}_{(aq)} + 2\text{e}^- \rightarrow \text{M}_{(s)}$

Voltaic vs electrolytic cells

- Voltaic = battery
- Energy conversion:
 - Voltaic is chemical energy (E) to electrical E
 - Electrolytic is electrical E to chemical E
- Direction of electron flow for both is anode to cathode

- Voltaic cells have the negative electrode as anode and positive as cathode
- Electrolytic has negative electrode as cathode and positive as anode
- Voltaic is spontaneous, electrolytic is non-spontaneous (meaning an external source of energy is needed, hence the symbol at the middle of the wire for diagram for electrolytic is a battery not a voltmeter)

Operation of electrolytic cells

- Is all in *one beaker*, electrodes are connected by power source (battery)
- Electrons are forced to flow by external power source from the weak reducing agent, the anode, to the weak oxidising agent, the cathode
- Anode is site of oxidation of anions: $Y^{2-} \rightarrow Y + 2e^-$
- Cathode is site of reduction of cations: $X^{2+} + 2e^- \rightarrow X$
- Uses inert electrodes usually

Key terms for Topic 9

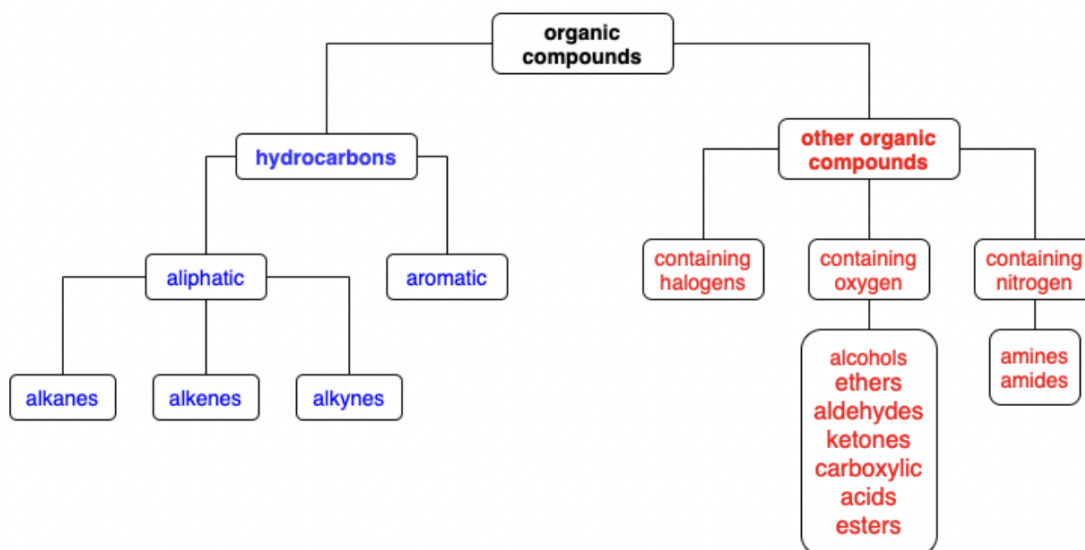
Term	Definition
Redox reactions	reactions that involve a transfer of electrons from one reactant to another
Oxidising agent (OA)	reactant that is reduced
Reducing agent (RA)	reactant that is oxidised
Oxidation state	charge for monatomic ions
Disproportionation reaction	a reaction in which the same element is oxidized and reduced at the same time
Endpoint	visible change in colour of titrated solution when an indicator is used - should be as close to equivalence point as possible
Equivalence point	when all moles of analyte have reacted with titrant

Topic 10: Organic chemistry

10.1 Fundamentals of organic chemistry

Organic chemistry overview

- In the broadest sense, Organic Chemistry is the study of carbon containing compounds.
- A somewhat more precise description is that OC is the study of covalently bonded compounds containing carbon, excluding carbonates and oxides
- Carbon is versatile and can be found in many compounds because:
 - 1) Carbon atoms can form 4 bonds
 - 2) Carbon atoms can form single, double or triple bonds
 - 3) Carbon atoms can join together to form long straight chains, branched chains and ring structures
 - 4) Carbon-carbon bonds are very stable (especially single C-C bonds), and are the most stable bonds in Group 14 of the Periodic Table
 - They have a high bond enthalpy (BE), which is the energy required to break one mole of a given bond type
- Classifications of organic compounds:



Functional groups

- Organic compounds are separated into classes based on their functional group
- A functional group is a site of reactivity in a molecule- memorize this for exams

- A class of molecules are molecules with the same functional group and similar chemical reactivity
- The classes can be seen in the diagram above: alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, aldehydes, ketones, carboxylic acids, esters, amines, amides, and also nitriles (nitriles are not in the diagram but they are also compounds containing nitrogen, alongside amines and amides)

Basic naming of organic compounds

1. The base name for all organic compounds contains a stem and a suffix
 - The stem tells you how many carbons is in the longest chain; this shows the “main part” of the compound
 - The suffix indicates what class the compound is
 - Eg alkanes have an “-ane” suffix, alkenes have an “-ene”, etc

Stems: number of carbons vs stem name

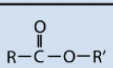
One carbon	Meth
Two	Eth
Three	Prop
Four	But
Five	Pent
Six	Hex
Seven	Hept
Eight	Oct

2. Organic compounds can be straight (or linear) chain molecules, or they may be branched molecules. There are extra steps when naming a branched compound.
 - a. Identify the longest continuous chain of carbon atoms and the branches (or side chains). The longest chain is the “main part” that you can find the “base name” from. However, if it is a compound with a functional group such as alkenes, alkynes- anything other than alkanes which has no functional group- the main branch MUST contain the functional group, even if its inclusion means the carbon chain identified is no longer the longest.

- b. Identify the side branch type using “stem + yl”, with the “stem” indicating the number of carbons in the branch
 - c. Identify the location of the side branch by numbering the carbon atoms in the longest chain, starting at the end closest to the branch or at the functional group, if there is a functional group present (alkanes have no functional group)
 - d. Name the side branch showing its location and type, putting a hyphen between the number and the type, with the number in front
- Eg “2-methyl”
 - e. Place the base name behind that of the side chain
3. There may be more than one branch.
 - a. If there are two or more of the same type of branch - add a prefix to the stem to show how many of that type of branch are present, AND include the locations of each branch
 - b. If there are two or more different types of branches, arrange their names (#+stem+yl) in alphabetical order before the base name
4. Some hydrocarbons are cyclic hydrocarbons, where the carbon atoms form a ring. Name the cyclic alkane by putting “cyclo” before the base name.

Each organic compound has its own suffix and unique naming method. This can be found below.

IUPAC naming of organic compounds

Compound Class (Homologous Series)	General Molecular Formula	Functional Group Structure	Functional Group Name	Example with condensed formula
HYDROCARBONS				
alkanes	C_nH_{2n+2}	n/a	n/a	C_4H_{10} $CH_3CH_2CH_2CH_3$ = butane
cycloalkanes	C_nH_{2n}	n/a	n/a	C_4H_8  = cyclobutane
alkenes	C_nH_{2n}	C=C	alkenyl	C_4H_8 $CH_3CH=CHCH_3$ = but-2-ene
alkynes	C_nH_{2n-2}	$C\equiv C$	alkynyl	C_4H_6 $CH_3C\equiv CCH_3$ = but-2-yne
arenes			phenyl	C_7H_8 $C_6H_5CH_3$ = methylbenzene
OTHER ORGANIC COMPOUNDS				
halogenated alkanes	$C_nH_{2n+1}X$	X (any halogen)	fluoro / chloro / bromo / iodo	C_2H_5I CH_3CH_2I = iodoethane
alcohols	$C_nH_{2n+2}O$		hydroxyl	C_3H_8O $CH_3CH_2CH_2OH$ = propan-1-ol
ethers	$C_nH_{2n+2}O$		ether	C_3H_8O $CH_3CH_2OCH_3$ = methoxyethane
aldehydes	$C_nH_{2n}O$		carbonyl	C_3H_6O CH_3CH_2CHO = propanal
ketones	$C_nH_{2n}O$		carbonyl	C_3H_6O CH_3COCH_3 = propanone
carboxylic acids	$C_nH_{2n}O_2$		carboxyl	$C_3H_6O_2$ CH_3CH_2COOH = propanoic acid
esters	$C_nH_{2n}O_2$		ester	$C_3H_6O_2$ CH_3COOCH_3 = methyl ethanoate
amines (primary)*	$C_nH_{2n+3}N$		amino	C_2H_7N $CH_3CH_2NH_2$ = ethylamine
amides (primary)*	$C_nH_{2n+1}ON$		amide	C_2H_5ON CH_3CONH_2 = ethanamide
nitriles	$C_nH_{2n-1}N$	$R-C\equiv N$	nitrile	C_2H_3N CH_3CN = ethanenitrile

- Note that for halogenoalkanes, amines and alcohols, there are three types: primary, secondary and tertiary
 - If the carbon that the functional group is bonded with is connected to only one other carbon, it is primary. If 2 carbons, secondary. And if 3, tertiary.

Structural formulas (SFs), empirical and molecular formulas

Molecular formulas simply show the number of each type of atom present in a compound.

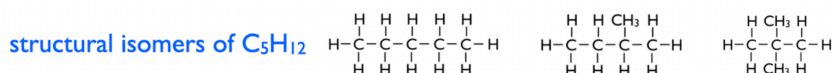
Empirical formulas show the lowest ratio of each element in a compound.
Structural formulas show the arrangement of the atoms and the bonds.

type of structural formula	butane	2,2-dimethylbutane
complete SF - shows all atoms + all bonds - remember that C atoms form 4 bonds!	$\begin{array}{cccc} \text{H} & \text{H} & \text{H} & \text{H} \\ & & & \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ & & & \\ \text{H} & \text{H} & \text{H} & \text{H} \end{array}$	$\begin{array}{cccc} \text{H} & \text{CH}_3 & \text{H} & \text{H} \\ & & & \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ & & & \\ \text{H} & \text{CH}_3 & \text{H} & \text{H} \end{array}$
condensed SF - no bonds shown, but groups of atoms listed in sequence - branches are shown in parentheses following the atom they are bonded to	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	$\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_3$
skeletal SF - only shows carbon-carbon bonds (or a few other types) - no C or H atoms shown		
stereochemical SF - shows the 3D arrangement of atoms - more on this in HL seminar and in the Bonding unit		

Structural Isomers

- Molecules with the same molecular formula but different structural formulas are called isomers
- They are called structural isomers when the structural formula is different due to changes in bonding patterns

Eg:



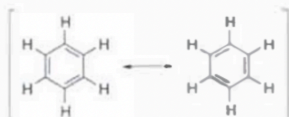
Saturated and unsaturated compounds

- Saturated compounds are organic compounds with only single carbon bonds
- Unsaturated compounds are organic compounds with double/triple carbon bonds
- Alkanes are saturated hydrocarbons
 - Single C-C bonds

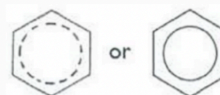
- Maximum number of H atoms attached to each C atom
- Alkenes, alkynes and benzene are unsaturated compounds
 - Double, triple, C-C bonds
 - Less-than-maximum number of H atoms attached to each C atom
- Benzene is an aromatic, unsaturated hydrocarbon that is very stable due to delocalized electron structure

The Importance of Delocalized Electrons and Resonance Structures

Benzene has a
RESONANCE
structure.



which can be
written as



The electrons that form the “second bond” in a C=C double bond do not pair up to form alternating single and double bonds.

(HL: You should know the “second bond” in the double bond is referred to as the π bond.)

Instead, these electrons are **delocalized** and spread out over all 6 carbon atoms in the benzene ring.

This is a **very stable** electron arrangement.

Homologous series

A **homologous series** is a group of organic chemicals with:

- | | |
|--|--|
| 1. the same general formula and the same functional group | e.g. alkenes = C_nH_{2n}
(all have 1 C=C double bond) |
| 2. successive members differ by CH₂ | e.g. first 4 members of the alkenes:
C_2H_4 C_3H_6 C_4H_8 C_5H_{10} |
| 3. chemical properties are the same for all members | e.g. all alkenes are combustible and react readily with bromine |
| 4. physical properties gradually change as you move along the homologous series | e.g. the boiling points of the alkenes increase as chain length increases |

- The reasoning behind the increasing boiling point has to do with London Dispersion Forces, found in Topic 4

combustion contribute towards a form of air pollution called particulates which can damage the respiratory tract and contribute to the formation of smog

Alkane reactions

- Substitution reactions
 - Where an atom / functional group on a molecule is replaced with another atom or functional group
 - Substitution of alkanes requires special conditions to overcome the low reactivity and stability
 1. Formation of reactive free radical intermediates
 2. Using high energy UV light to form free radicals
- Why alkanes are stable with low reactivity:
 1. High BE (bond enthalpy) of C-C and C-H bonds
 - a. So alkanes will only react if there is a strong source of E to break the bonds
 2. Non-polar nature
 - a. Lack of a polar region on molecules makes it less likely to react with the most common reactants

Free radical substitution reaction mechanism

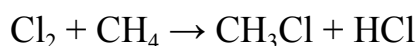
Steps for halogenation of alkanes

1. Initiation
 - Breaking the bond in the halogen molecule requires energy of UV light
 - When the bond between halogen atoms break, it is homolytic fission; one electron from the shared bonding electron pair (BEP) stays with each atom- there is an even split
 - Particles with an odd number of electrons or unpaired electrons are very reactive and are called free radicals
 - $\text{CH}_4 + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{HCl}$
2. Propagation
 - Each step uses a free radical and produces a different free radical
 - a. $\text{CH}_4 + \text{Cl}\cdot \rightarrow \text{CH}_3\cdot + \text{HCl}$
 - One of the products of the overall reaction (rxn) is produced along with a new free radical to be used in step (b)
 - b. $\text{CH}_3\cdot + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{Cl}\cdot$
 - Other product of overall rxn forms, also the chlorine free radical reforms so step 2 can continue, leading to chain rxn
3. Termination
 - 2 free radicals combine in this stage, removing the free radicals and stopping the chain rxn from continuing
 - $\text{Cl}\cdot + \text{Cl}\cdot \rightarrow \text{Cl}_2$

- $\text{Cl}\cdot + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{Cl}$
- $\text{CH}_3\cdot + \text{CH}_3\cdot \rightarrow \text{C}_2\text{H}_6$

Overall:

1. $\text{Cl}_2 \xrightarrow{\text{uv light}} \text{Cl}\cdot + \text{Cl}\cdot$ initiation
2. $\text{CH}_4 + \text{Cl}\cdot \rightarrow \text{CH}_3\cdot + \text{HCl}$ (x2) propagation
3. $\text{CH}_3\cdot + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{Cl}\cdot$ (x2)
4. $\text{Cl}\cdot + \text{Cl}\cdot \rightarrow \text{Cl}_2$ or termination
 $\text{Cl}\cdot + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{Cl}$ or
 $\text{CH}_3\cdot + \text{CH}_3\cdot \rightarrow \text{C}_2\text{H}_6$



Combustion vs selective oxidation of alcohols

*definitions of redox terms can be found in Topic 9

- Combustion rxns are a type of oxidation rxn
 - The carbons are oxidised
 - O_2 is a very strong OA
- Combustion = complete oxidation since all C atoms fully oxidized to CO_2 (ox state +4)
 - More E is released when CO_2 forms rather than CO
 - Energy is released when bonds form
 - BE for 2 C=O in CO_2 is greater than that of the 1 C-O triple bond in CO
- Selective oxidation is when only a few of the carbon atoms undergo oxidation in the presence of OAs that aren't O_2 , denoted by [O]
 - Selective oxidation rxns convert one type of OC into another

Common oxidizing agent (OA) for alcohol oxidations

- Acidified potassium dichromate ($\text{H}^+/\text{K}_2\text{Cr}_2\text{O}_7$) is the OA used in many selective oxidation reactions; the $\text{Cr}_2\text{O}_7^{2-}$ is the OA
- It must be acidified first by adding some sulfuric acid
- Acidified potassium dichromate is represented by $\text{H}^+ / \text{Cr}_2\text{O}_7^{2-}$
- $\text{K}_2\text{Cr}_2\text{O}_7$ is orange, in ox of alcohol will be reduced to green Cr^{3+}

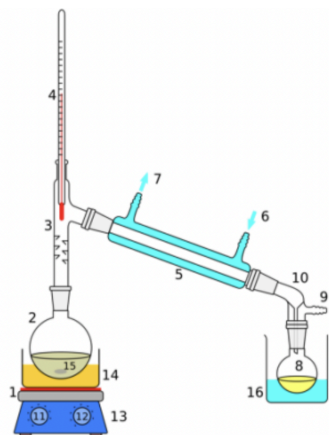
Selective oxidation of alcohols + reaction conditions

- 1° alcohols
 - 1° alcohol + [O] $\rightarrow$ aldehyde
 - Example: oxidation of ethanol to ethanal under distillation conditions
 1. As long as temp of rxn mixture in the flask being heated is under 75°C , only ethanal will vapourize
 2. The vapour (ethanal) rises into fractionating column (directly above the flask) then moves into the condenser (to the side)

of the flask, “side tunnel” that runs from the flask to a different container)

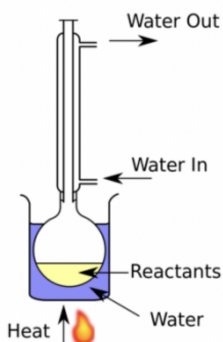
3. Cold H₂O surrounding the condenser decreases the temp of aldehyde vapour turning it into liquid
4. Purified liquid aldehyde is collected in a second flask
- Distillation takes advantage of the different boiling points (BPs) of substances; aldehydes have a lower BP than alcohols and carboxylic acids

distillation apparatus



- Aldehyde + [O] → carboxylic acid
 - Reflux is vaporisation followed by condensation, which allows prolonged heating of a substance without it boiling dry
 - Further oxidation of the aldehyde to carboxylic acid by reflux
 1. As in distillation, the aldehyde evaporates and aldehyde vapour rises
 2. In the condensing tube positioned above the rxn vessel, the aldehyde vapour turns into liquid, and this condensed liquid is returned to the rxn mixture
 3. The aldehyde that returns to the rxn mixture is now in further contact with the OA, pushing the rxn further to form carboxylic acid

reflux apparatus



- 2° alcohols
 - 2° alcohol + [O] → ketone + [O]

- The C-C and C=O bonds in ketone are too strong to break, so no further oxidation rxn with O atoms can occur once a 2° alcohol becomes a ketone
- 3° alcohols
 - Cannot be oxidised
 - Because the C-C bonds are too strong, thus preventing the formation of C=O bonds

Esterification reactions

Carboxylic acid + alcohol → ester + water

- With the OH on the R-COOH and the H on the HO-R being attracted to each other
- Requires catalyst of concentrated H₂SO₄ and heat
- In diagrams, draw reactants so functional groups “face” each other

Saturated vs unsaturated hydrocarbons

- Alkanes are saturated hydrocarbons
 - Single C-C bonds (no pi bonds only sigma)
 - Maximum H attached to each C atom
- Alkenes, alkynes and benzene are unsaturated compounds
 - Double, triple, C-C bonds (with pi bonds)
 - Less-than-maximum H attached to each C atom

Alkanes vs alkenes

- Alkanes are more reactive than alkenes
 - The double C=C bond in alkenes is a site of reactivity due to the high electron density (attracts electrophiles)
 - When alkenes react (other than O₂ combustion), only one of the C=C bond breaks; the pi bond, not the sigma bond
 - This bond (the pi bond) has less BE than a singular C-C bond, so it's easier to break, making it easier for alkenes to react than alkanes
- Alkanes have combustion rxns and free radical substitution rxns
- Alkenes have addition rxns (hydrogenation, halogenation, hydration, polymerization)

Addition reactions with alkenes

- Addition rxns happen when an atom / group of atoms is added to each C atom in C=C double bond; the pi bond breaks in the double bond
 - The unsaturated compound becomes saturated

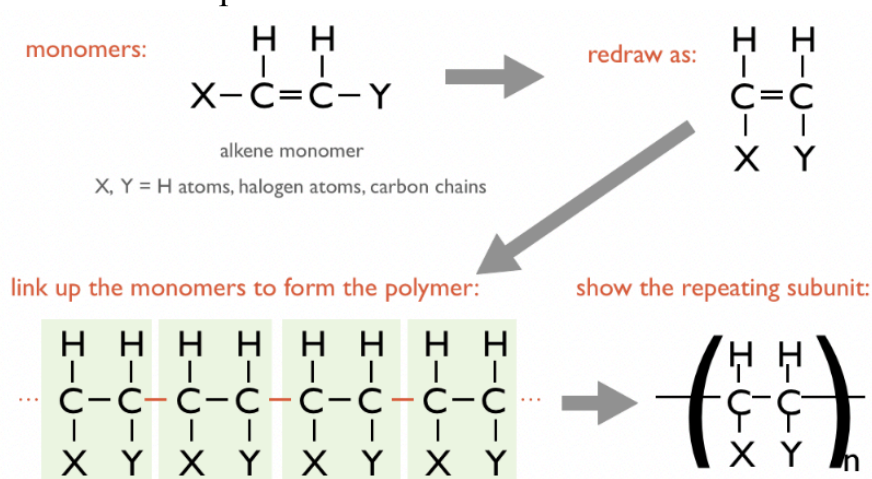
Adding	Rxn name	Product	Conditions
--------	----------	---------	------------

H ₂	Hydrogenation	Alkane	Ni, 150°C
Halogen	Halogenation	Dihalogenoalkane	none
Halogen hydride		Halogenoalkane	none
H ₂ O	Hydration	Alcohol	H ₂ SO ₄ Heat with steam
_____	Polymerization	Long-ass chain	_____

- Addition reactions with Br₂ can be used to test for unsaturation
 - Br₂ is reddish brown liquid
 - When the Br-Br bond breaks during addition rxn with unsaturated compound, the reddish-brown colour disappears (become colourless)
 - Alkanes don't react, so the brown colour remains
 - Alkenes do react, so the solution become colourless

Addition polymerisation

- Addition polymers are made by breaking one of the C=C bonds (pi) in the monomers, and joining monomers together
 - Eg polypropene
- General pattern:



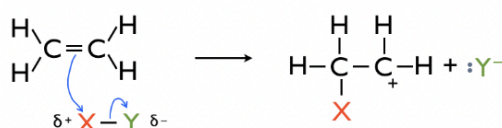
Electrophilic addition reactions for alkenes

- Turns an alkene into a saturated compound
- C=C bond is quite reactive
 - C atoms are sp² hybridised

- Double bond is electron dense
- Pi bond is area of electron density, hence it attracts electrophiles and has a polarising effect on dihalogens
- The pi bond is also weak and less tightly held, as pi bond electrons are overlapping side by side both above and below the internuclear axis
- Electrophile examples
 1. Hydrogen halides
 2. Halogens
 3. Interhalogens
- Rxn mechanism

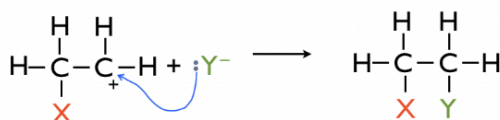
Step 1: Electrophilic attack and formation of a carbocation

slow step



Step 2: Formation of bond between carbocation and the halide ion

fast step



Markovnikov's rule

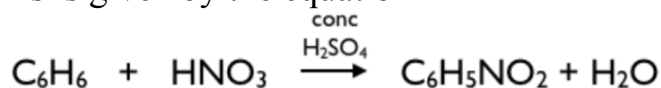
- The formation of a secondary carbocation is more stable than a primary carbocation
- In the addition rxns of asymmetrical alkanes (when different numbers of C atoms are on each side of C=C bond), 2 organic products are possible but only 1 is favoured
 - Favoured = major product, otherwise is minor
- In the favoured product, the halogen bonds to the most stable carbocation
 - High concentration of positive charge on a C atom makes it unstable
 - Alkyl groups bonded to the carbocation have a positive inductive effect (small electron donating effect), thus “pushing” electrons towards the carbocation, reducing the density of the + charge on the carbocation
 - 1° carbocation has only 1 positive inductive effect = least stable
 - 2° carbocation more stable, 2 effects
 - 3° has 3 effects, most stable
- The electrophilic atom bonds to the C atom with the most inductive effects

Benzene

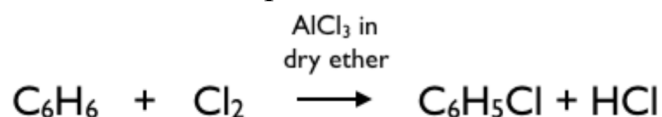
- Benzene is unsaturated but does not undergo addition easily due to the presence of already having the resonance structure with delocalized electron which is already a very stable electron arrangement, which addition rxns would disrupt
 - If C=C changes to C-C as in addition rxns, the delocalized electrons would now only spread out over 4 C atoms which is less stable as there is more electron-electron repulsion
 - So an addition rxn would disrupt resonance structure, which is not energetically favourable
- Hence substitution rxns which maintain the delocalization of electrons over 6 C atoms are more preferred for benzene

Electrophilic sub of benzene

- An electrophile (E^+) replaces an atom / group on benzene ring
- Electrophiles are electron deficient species with + charge, attracted to electron rich regions
- An example is the nitration of benzene
- This is given by the equation



- Alternatively, a halogen can be added onto benzene in a substitution reaction. An example is:



Nucleophilic substitution of halogenoalkanes

- Nucleophile:
 - Electron rich species attracted to areas of electron deficiency
 - An electron rich region on a nucleophile will be attracted to the electron deficient C atom bonded to the halogen
 - Electrons shift from C atom to the halogen due to the high EN of the halogen
- Halogenoalkanes can undergo nucleophilic sub where a nucleophile replaces the halogen in the halogenoalkane
 - Halide ion removed is called leaving group
 - Halogenoalkane + hydroxide ion $\rightarrow$ alcohol + halide ion
- Primary halogenoalkanes produce primary alcohols

Some equations for nucleophilic sub using $\text{NaOH}_{(\text{aq})}$

Complete: $\text{CH}_3\text{Br} + \text{NaOH} \rightarrow \text{CH}_3\text{OH} + \text{NaBr}$

Ionic: $\text{CH}_3\text{Br} + \text{Na}^+ + \text{OH}^- \rightarrow \text{CH}_3\text{OH} + \text{Na}^+ + \text{Br}^-$

Net ionic: $\text{CH}_3\text{Br} + \text{OH}^- \rightarrow \text{CH}_3\text{OH} + \text{Br}^-$

Key terms for Topic 10

Term	Definition
Organic chemistry	the study of covalently bonded compounds containing carbon, excluding carbonates and oxides
Functional group	a site of reactivity in a molecule
Class (of molecules)	molecules with the same functional group and similar chemical reactivity
Molecular formulas	the number of each type of atom present in a compound
Empirical formulas	the lowest ratio of each element in a compound
Structural formulas	the arrangement of the atoms and the bonds
Isomers	molecules with the same molecular formula but different structural formulas
Structural isomers	isomers where the structural formula is different due to changes in bonding patterns
Saturated compounds	organic compounds with only single carbon bonds
Unsaturated compounds	organic compounds with double/triple carbon bonds
Benzene	an aromatic, unsaturated hydrocarbon that is very stable due to delocalized electron structure
Homologous series	a group of chemicals with the same general formula and functional group, same chemical properties, with each successive member differing by CH_2
Complete	occur in presence of excess O_2

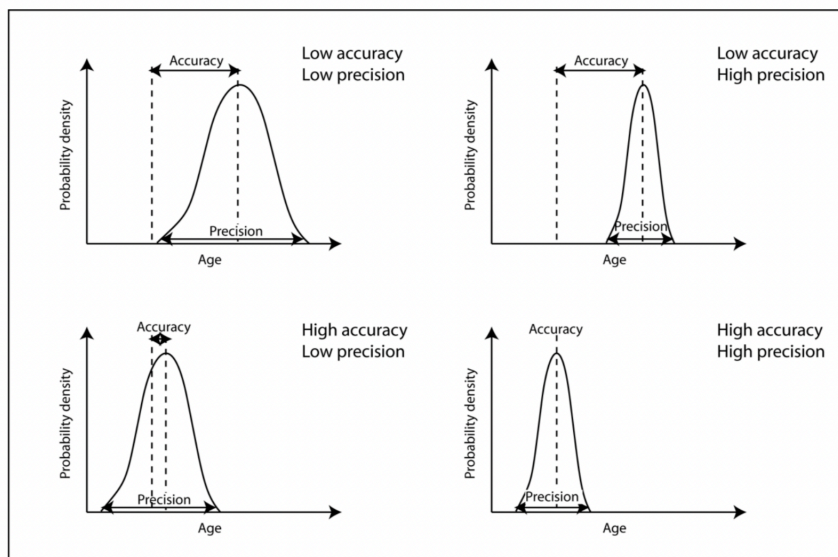
combustion reactions	
Incomplete combustion reactions	occur in presence of limited O ₂
Substitution reactions	where an atom / functional group on a molecule is replaced with another atom or functional group
Reflux	vaporisation followed by condensation, which allows prolonged heating of a substance without it boiling dry
Markovnikov's rule	formation of secondary carbocations are more stable than primary carbocations
Electrophiles	electron deficient species with positive charge, attracted to electron rich regions
Nucleophile	electron rich species attracted to areas of electron deficiency

Topic 11: Measurement and data processing

11.1 Uncertainties and errors in measurement and results

- Quantitative data is obtained from measurements- the uncertainties/errors associated with those measurements, determined by the apparatus and human error (but never write human error in a lab report!), will affect the final result
- Propagation of these errors shows the impact of them on the final result
 - Error propagation of measurement uncertainties derived from the uncertainty written on the lab apparatus will be useful in IAs- mainly the chemistry IA
- Experimental error in a result is the difference between the measured (or calculated) value and the accepted (correct) value.
- Measurement uncertainty is the potential error derived from the equipment used, and should be written as ($\pm$ ____) next to the measurement recorded
 - There is absolute uncertainty, which is the number itself, and percentage uncertainty- calculated by
$$\left(\frac{\text{absolute uncertainty}}{\text{measurement recorded}} \right) \times 100\%$$
- There are two types of error: systematic and random. Systematic errors are associated with a loss of accuracy, whereas random errors are associated with loss of precision.
 - Accuracy refers to how close a measurement (or calculated value) is to the true value
 - Precision refers to how close several experimental measurements of a value are to each other

Accuracy vs Precision in Sets of Data



- Systematic error always causes the experimental value to be skewed in one direction relative to the expected value - hence affecting the **accuracy**
 - i.e. always too high, or always too low as compared to the expected result
 - This type of error results from a flaw in the experimental procedure (or design) or equipment flaw
 - This error can only be reduced by careful experimental design, but cannot be reduced by repeating the experiment
- Random error causes the experimental value to vary from the experimental value in either direction; both higher and lower than the expected value - hence affecting **precision**
 - Results from measurement uncertainty of equipment, variability in surroundings that affects readings, observer misinterpretation
 - May be reduced by repeating measurements
- In a lab report, always use the words “random” or “systematic” error - human error should never make its way into a report! When instances of human error occur, the experiment should be re-done, as “human error” indicates a **mistake**, and no examiner likes to see that!
- A calculation that may prove useful in Paper 3 and in lab reports is percentage error:

Percent Error

$$\% \text{ error} = \left(\frac{\text{experimental value} - \text{accepted value}}{\text{accepted value}} \right) \times 100$$

Whenever you calculate any value in experiment, you must always compare it to the “accepted” value (aka “literature” value, “true” value).

Only use the AVERAGE experimental value when you find the % error.

11.2 Graphical techniques

- Graphs are a useful tool by which to see the relationship between the independent and dependent variables
 - You should already know (from before DP) terms such as “positive linear”, “negative linear”, “quadratic”, “exponential” etc
 - Use these terms to describe the relationship shown in your graph in your IA
- Sketched graphs have labelled but unscaled axes, and are used to show qualitative trends
- Drawn graphs have labelled and scales axes, and are used in quantitative measurements
- You should already know (from before DP) how to produce trendlines and error bars on graphs in Excel or another similar software, and how to calculate slope and y-intercept as well as their significance.
 - These skills will be used in lab reports, most notably in your IA

11.3 Spectroscopic identification of organic compounds

Index of Hydrogen Deficiency (IHD)

- A measurement of the degree of unsaturation of a compound
 - Saturated compounds: all C atoms are singly bonded to 4 other atoms
 - Unsaturated compounds: 1 or more C atoms have a double/triple bond with another atom

- IHD is the number of H₂ molecules needed to convert a saturated molecule into its corresponding non-cyclic saturated equivalent
- IHD from structures:
 - Double bond = 1
 - Triple bond = 2
 - Non-aromatic ring = 1
 - Benzene ring = 4
- IHD from molecular formulas:
 - $C_cH_hN_nO_oX_x$
 - $(0.5) \times (2C + 2 - H - X + N)$

Principles of Spectroscopy

- Molecules can absorb different forms of electromagnetic (EM) radiation
- Different forms of EM radiation interact with atoms differently, and are used in different techniques

Gamma rays	X-rays	UV & visible	Infrared light	Microwaves	Radio waves
Interacts with nucleus	Interacts with inner e-	Interacts with valence e-	Affects vibration of molecules	Affects rotation of molecules	Affects spin of nuclei
Not used in analysis	Crystal lattice structure	e-transitions between E levels	Types of chem bonds	Bond lengths	Environment around atoms in a molecule (NMR)

Some equations:

- $c = f\lambda$ $E = hf$ $E = \frac{hc}{\lambda}$
 - Units: c (m s⁻¹), f (Hz or s⁻¹), λ (m), E (J)
- Wavenumber
 - Common unit used in spectroscopy
 - Is reciprocal of wavelength ($\frac{1}{\lambda}$)
 - Measured in cm⁻¹

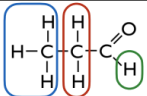
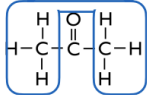
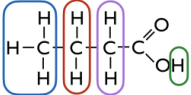
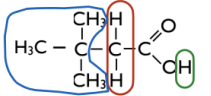
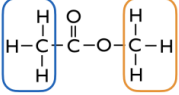
Infrared Radiation (IR) Spectra

- Diff chem bonds in molecules vibrate at diff frequencies and only absorb radiation with a corresponding frequency/wavelength
 - Radiation absorbed by vibrating chem bonds found in IR region of EM spectrum
- IR radiation absorption
 - Helps in identification of molecules
 - Responsible for greenhouse effect
- Only polar bonds (not necessarily polar molecules) absorb IR radiation
- IR absorption only happens when a bond vibration produces a change in dipole moment
 - Non-polar bond: no bond dipole at any length, so IR inactive
 - Polar bond: change in bond length changes strength of bond dipole, IR active
- Bond stretching/bonding must change the dipole moment of the molecule in order for IR absorption
- The lower the y-axis (% transmission), the greater the absorption of IR radiation
- Fingerprint region
 - Occurs between $400\text{--}1400\text{ cm}^{-1}$
 - Very complex spectral pattern
 - Unique for each compound (except enantiomers)
 - Can be used to identify unknown compounds by comparison of region with library of known compounds
 - Propan-1-ol and propan-2-ol have same spectral patterns outside the fingerprint region, so that region of the IR spectrum cannot distinguish between isomers
- Table 26 has IR absorption data
 - Broad signal at $3200\text{--}3500$: O-H bond in alcohols
 - Broad signal at ~ 3000 : O-H in carboxylic acids
 - Sharp signal at 2900 : C-H bonds
 - Very sharp signal at 1700 : C=O bonds

Nuclear Magnetic Resonance (^1H NMR) Spectroscopy

- Applications: MRI scans
- Region of EMS used: radio waves
 - Very low E radiation so non-invasive

- How it works:
 - H atoms in molecules interact with radiowaves in a magnetic field
 - Depending on the chemical environment, the nuclei in the H atoms will absorb different amounts of E in the radiowave region of the EMS
- ^1H NMR tells us the number of chemical environments for H atoms and the #H atoms in each environment
 - Chem env relates to where atom in molecule and neighbors
- Chem environments:

compound	structural formula	# chemical environments	ratio of H atoms
propanal		3	3:2:1
propanone		1	n/a
butanoic acid		4	3:2:2:1
3,3-dimethyl butanoic acid		3	9:2:1
methyl ethanoate		2	3:3

- Key features:
 - Number of signals (peaks) = # diff chem env
 - Peaks correspond to radiowave E absorbed by protons in diff chem env
 - Relative area under each signal = ratio of H atoms in each env
 - Chemical shift = type of proton (Table 27) (position of H atom)
 - Integration trace = relative area = #H in each env

Mass spectrometry (MS)

- Can be used to determine:
 1. Natural abundance of isotopes of an element
 2. Structure of molecules
- Mass spectra gives information about the fragments formed when an organic compounds (OC) breaks into smaller pieces
 - Peaks = fragments of molecule
 - m/z = mass charge ratio

- Most fragments have a charge of +1
 - If no charge, WILL NOT BE PRESENT ON SPECTRUM
- Molecular ion (M^+)
 - Sample M is introduced into the mass spectrometer and bombarded with high speed electrons that knock out an electron from the molecule
 - $M + e^- \rightarrow M^+ + 2e^-$
 - (molecule)⁺
 - Is usually peak with highest m/z value on spectrum
 - Will breakdown to produce one charged and one uncharged fragment with only the charged one showing on the spectrum
 - Splits by fragments giving most stable ion forms
- Analyzing mass spectra:
 1. Find M^+ and M_r
 2. Find MF (using EF and M_r)
 3. Look at mass differences of fragments to determine what is lost from the M^+ then deduce formula of fragment on spectrum (what is still present after losing fragment from M^+)
 - Mass difference = $M_r - (m/z \text{ of fragment on graph})$
 4. Determine structural formula
 - Matching fragments that are possible to make from the mass spectrum to the possible structures

Key terms for Topic 11

Term	Definition
Quantitative data	data obtained from measurements; numerical data
Experimental error	the difference between the measured (or calculated) value and the accepted (correct) value
Measurement uncertainty	the uncertainty/error derived from the equipment used
Accuracy	how close a measurement (or calculated value) is to the true value
Precision	how close several experimental measurements of a value are to each other

IHD	a measurement of the degree of unsaturation of a compound
Wavenumber	common unit used in spectroscopy, is reciprocal of wavelength
IR Spectra	used to determine functional groups in molecules
¹ H NMR Spectroscopy	used to identify the structure of organic compounds
MS	gives information about the fragments formed when an OC breaks into smaller pieces