

AQA AS level Unit 1 Chemistry notes by Luna Hu

Atomic structure

Particle	Mass (kg)	Relative mass	Charge (c)	Relative charge
Proton	1.67×10^{-27}	1	1.6×10^{-19}	+1
Neutron	1.675×10^{-27}	1	0	0
Electron	9.11×10^{-31}	1/1840	-1.6×10^{-19}	-1

Relative atomic mass: Average weighted mass of an atom of an element relative to 1/12 mass of an atom of C12
 → This is why mass of C12 is exactly 12.00000 – it is the reference isotope.

Relative molecular mass: Mass of a molecule relative to 1/12th mass of C12 atom. [**Relative formula mass for ionic**]

Isotope: atoms with the same number of protons but different number of neutrons.

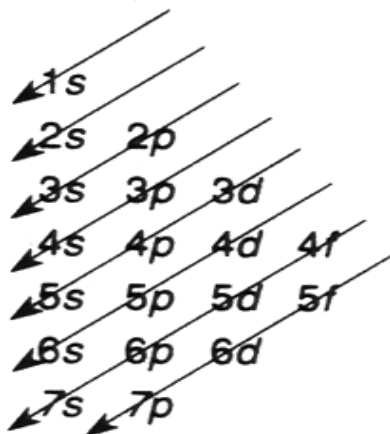
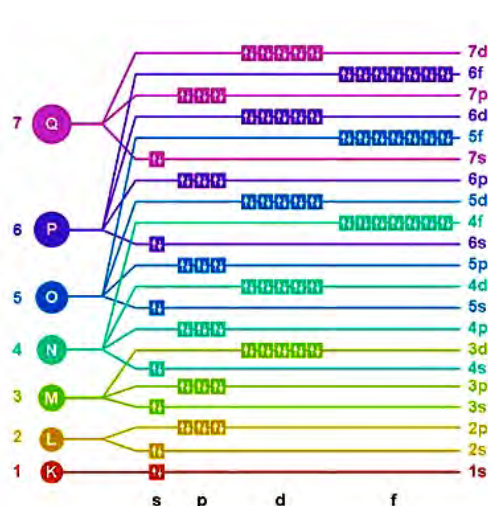
→ Isotopes have similar chemical properties as they have the same electron number and configuration, which determines chemical property.

Mass spectrometer:

- Find out relative atomic mass, relative molecular mass, relative isotopic abundance, and molecular structure and to identify elements.

Condition: vacuum – no obstruction, lower pressure (thus less heat required to vaporize sample) and to clean out sample.

- Vaporization** – Sample is vaporized so there is no attraction between the atoms.
- Ionization** – high-energy electrons from an electron gun knocks out electron(s) thus ionizes gaseous sample (in order for the following events to happen)
- Acceleration** – negatively charged plates attract the ionized sample, forcing the sample through slits, forming a Cation beam.
- Deflection** – The Cation beam is deflected by the magnetic field, as it is electrically charged. Extent of deflection depends on the m/z ratio → this ensures 1 isotope detected each time.
- Detection** – The sample lands on negatively charged detection plate, accepts electron(s), and a current passes. The current is proportional to the abundance of the isotope. (Small peaks far away from main peaks are caused by 2+ ions in which 2 electrons have been removed)
 → Generate a mass spectrum showing the relative abundance against m/z ratio.



Electron arrangements:

Main levels: 1, 2, 3, 4, etc.

Sub levels: s, p, d, and f orbitals.

The atomic orbital is the area where electrons have a 95% chance of being found. Each orbital holds up to 2 electrons. (Pauli exclusion principle)

*4s is of lower energy than 3d at neutral state thus is filled before 3d. It is also removed first when ionized!

In p orbital, separate orbitals are filled first before the electrons start pairing up because they repel.

Tip: use noble gas shorthand while writing electronic structures and watch out for ions!

Ionization energy: The amount of energy required to remove 1 mole of electrons from 1 mole of gaseous atoms. (kJ mol^{-1})

Successive ionization energies: removing electrons one by one.

Trends in ionization energies:

Across a period: Increases, due to increased nuclear charge

∴ increased attraction between electrons and nucleus

∴ decreased atomic radii.

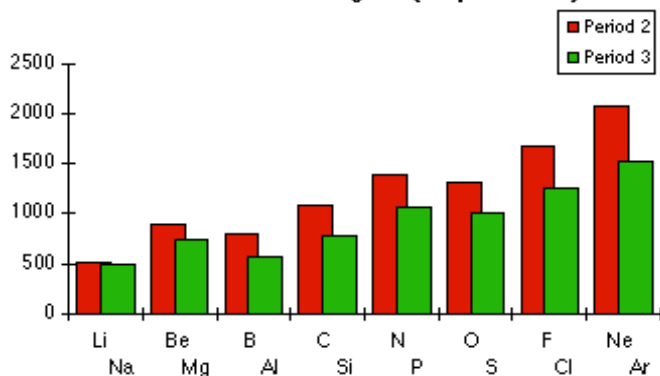
And since they are at same main energy level, the shielding is similar.

Down a group: decreases

- Increased shielding, shells and distance from outermost electrons to nucleus.

- Despite an increased nuclear charge

First ionisation energies (kJ per mole)



Deviations:

Aluminium: 3P orbital is of higher energy than 3S thus less energy is required to remove the outermost electron.

Sulfur: the electrons at the 3P orbital pairs up, they repel, thus energy required to remove the outermost electron is lowered.

This supports the theory of electron orbitals. (Due to the energy gaps.)

Successive ionization energy gets higher increasingly due to:

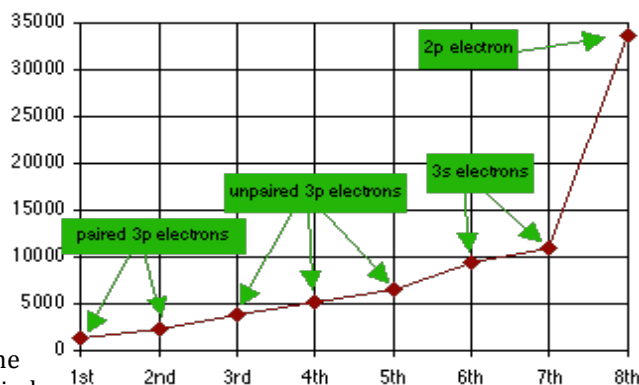
- Increased nuclear charge
 - smaller atomic radii.
- Thus increased attraction between outermost electron and nucleus

The big jumps in energy is caused by changes in energy level, be it sub or main. Energy Δ in main is larger; because energy required to remove an electron closer to nucleus (and with less shielding) is much higher.

* Data on successive energy level can be used to determine the group in which the element is.

Periodicity: the quality of character of being periodic or the tendency to recur at intervals. - Trends that occur across a period are repeated at each period.

The first 8 ionisation energies of chlorine (kJ per mole)

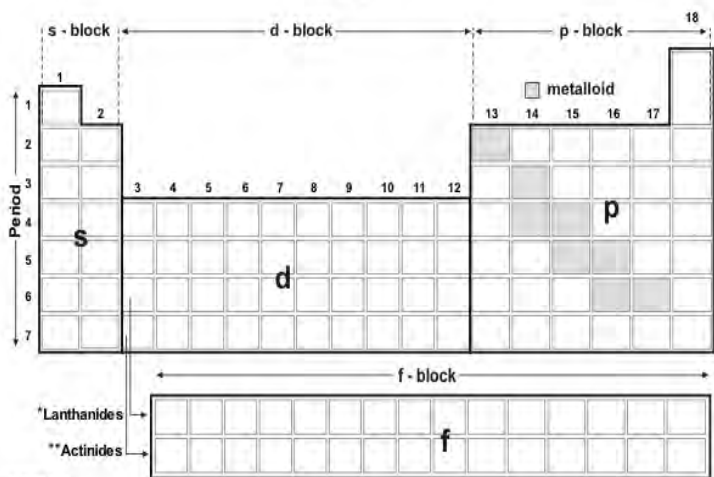


Periodic trends:

Group	1	2	3	4	5	6	7	0
Element	Sodium	Magnesium	Aluminium	Silicon	Phosphorus	Sulfur	Chlorine	Argon
Electron arrangement	[Ne] 3s ¹	[Ne] 3s ²	[Ne] 3s ² 3p ¹	[Ne] 3s ² 3p ²	[Ne] 3s ² 3p ³	[Ne] 3s ² 3p ⁴	[Ne] 3s ² 3p ⁵	[Ne] 3s ² 3p ⁶
	s-block		p-block					
	Metals			Semi-metal	Non-metals			Noble gas
Structure of element	Giant metallic			Macro-molecular (giant covalent)	Molecular			Atomic
					P ₄	S ₈	Cl ₂	Ar
Melting point, T _m / K	371	922	933	1683	317 (white)	392 (monoclinic)	172	84
Boiling point, T _b / K	1156	1380	2740	2628	553 (white)	718	238	87

Elements placed according to proton number
Blocks according to highest energy electron

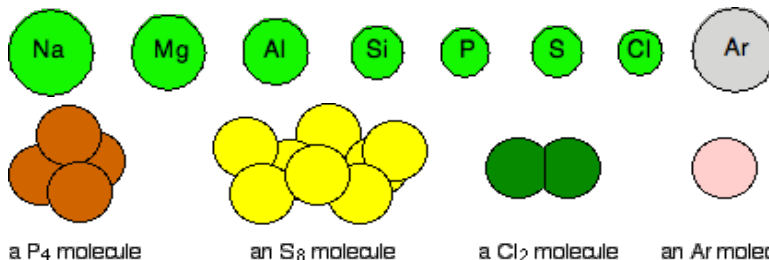
Group



MP and BP: depends on type of bonding.

- Atomic radii decreases - similar shielding + increased nuclear charge
- Conductivity: Increases then decreases → #delocalized electrons increases, then no free electrons.

Electronegativity (the ability of an atom to attract electron density towards itself in a covalent bond): increases
*increased nuclear charge *similar shielding *smaller atomic radii



MOLES

Mole is the system international standard unit of measurement for amount of substance. It is the number of atoms present in 12 grams of C12.

Ideal gas equation: $PV = nRT$

P: pressure (Pa)

V: Volume (m^3)

N: number of moles

R: $8.31 \text{ J K}^{-1} \text{ mol}^{-1}$ (given)

T: Temperature (K)

1 mole = 6.022×10^{23}
number of atoms.
A.K.A. Avogadro
constant/number

Volume		Pressure		Temperature
$\frac{\text{dm}^3}{1000} = \text{m}^3$	$\frac{\text{cm}^3}{1000000} = \text{m}^3$	kPa x 1000 = Pa	MPa x 1000000 = Pa	$^{\circ}\text{C} + 273 = \text{K}$

Empirical and molecular formulae:

- Find mass or percentage of each element.
- Divide each relative atomic mass
- Divide all by the smallest number (in step 2)
- Form simplest whole number ratio of atoms of each element present in a compound.
- If it is not a whole number e.g. $\frac{1}{2}$ multiple all by largest denominator.

Empirical formulae: simplest whole number ratio of atoms of the elements in a compound.

Molecular formulae: the actual amount of atoms of each element in a compound. (Usually a multiple of empirical formulae)

CONCENTRATION = MOLES / VOLUME

Atom economy: mass of desired product/total mass of reactants *100 (can be increased by selling byproducts)

Percentage yield: Actual yield/Theoretical yield *100

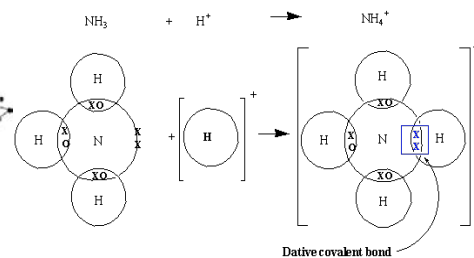
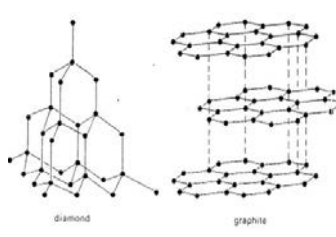
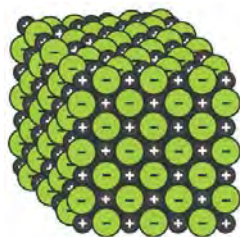
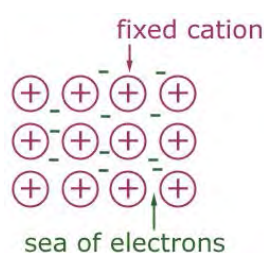
% Yield compares the amount produced compared to the amount you should get, whereas atom economy is the proportion of the mass of all the products that is the desired product(s) [i.e. could be sold for profit]

Difference in actual yield and theoretical yield may arise due to:

- Side reactions
- Products lost in isolation
- Incomplete reaction

Bonding & intramolecular forces

Type	Metallic	Ionic	Covalent (sharing of pair(s) of electrons)	
Structure	Giant metallic	Giant ionic	Macro-molecular	Simple covalent
Description	Strong electrostatic force of attraction between positive ions and sea of delocalized electrons	Transfer of outermost electron(s) to form 2 ions; strong electrostatic force of attraction between opposite charges.	Each atom in the structure is covalently bonded to adjacent atoms, which are difficult to break.	2+ atoms share pair(s) of electrons. Strong electrostatic force of attraction between the positive nuclei and the pair of electrons, but weak intermolecular force.
Features	<ul style="list-style-type: none"> • High BP • Malleable and ductile (no real bonds, can slide) • Insoluble due to strong bonds (except in other metals) • Conducts electricity because of delocalized electrons (which can move) 	<ul style="list-style-type: none"> • High BP • Brittle: if layers slide over, same charges meet and repel. • Maybe soluble in polar solvents but not in non-polar. • Conducts electricity when molten or dissolved. 	<ul style="list-style-type: none"> • High BP • Insoluble • Doesn't conduct electricity [EXCEPT GRAPHITE] → Weak VDW between layers of graphite; with delocalized electrons in between. 	<ul style="list-style-type: none"> • Low BP • Insoluble in polar solvents, maybe soluble in non-polar solvents. • Doesn't conduct electricity * Dative covalence: when 1 atom donates both of the electrons, (a lone pair) forming a charged molecule.



Structure and bonding of graphite:

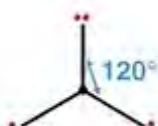
- Layers of carbon atoms
- Connected by strong covalent bonds within each layer (trigonal planar)
- Weak VDW forces between layers
- Many strong covalent bonds need to be broken (therefore high MP and BP)

Polar molecule: When there is a large difference in the electronegativity of the atoms of a covalent bond, resulting in $\delta+$ and $\delta-$.
Intermolecular forces:

Type	Van der waals	Dipole-dipole	Hydrogen
Description	Electrons are mobile <ul style="list-style-type: none"> • At any instant of time their distribution is uneven • $\delta+$ and $-$ ends induces dipole in surrounding molecules. 	<ul style="list-style-type: none"> • Uneven charge distribution due to large difference in electronegativity gives rise to a permanent dipole. • Molecules will adjust to give an arrangement where the molecules are attracting each other. 	When Hydrogen is bonded to a highly electronegative atom (Nitrogen, Oxygen, Fluorine) causing it to acquire significant positive charge Each atom H is attracted to has lone pair(s) H in 1 molecule is attracted to the lone pair of another molecule. (Strongest intermolecular force)
Increase strength	Longer Greater surface area More diffuse More electrons More shielding Larger nuclear charge	Larger difference in electronegativity	Water is one of the strongest because there is an equal number of Hydrogens and lone pairs of electrons. Ice floats on water because at solid state, the hydrogen bonds dominate, which aligns the H ₂ O molecules in such a way that it is less dense than liquid water.



Linear



Trigonal planar



Tetrahedral



Trigonal bipyramidal



Octahedral

Shape of molecules depends on number of electrons of central atom. Be it bonding pair or lone pair.

Electron pair repulsion theory: electrons want to be as far away from each other as possible to minimize repulsion.

$LL > LB > BB$ (strength of repulsion)

Each lone pair decrease angle by 2.5°

ORGANIC CHEMISTRY

Structural formula: Shows the arrangements of atoms and functional groups in molecules.

Displayed formula: (drawn out) Simplified model of compound showing bonds and atoms involved.

Homologous series: Same chemical properties (functional group), trend in physical properties and differs by CH₂

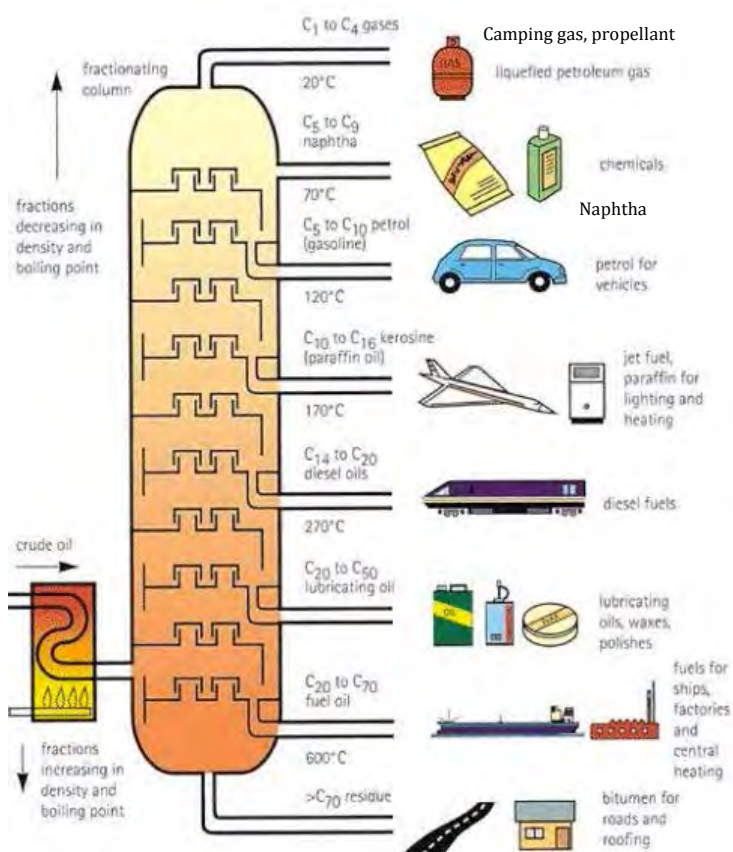
Functional groups: A portion of a molecule known to be responsible for the chemical characteristics of a particular compound.

Structural isomerism: Compounds with the same molecular formula but different structural formula.

Chain isomerism: Carbon chain is different (branching)

Position isomerism: Functional group placed on a different carbon

Functional group isomerism: Same molecular formulae, different functional groups.

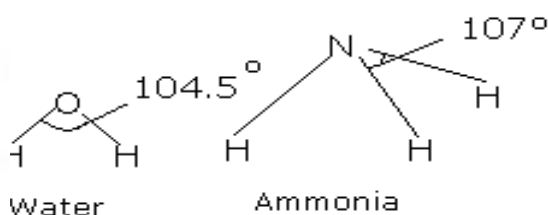


Alkanes – Saturated hydrocarbons (contains hydrogen and carbon only)

Petroleum is a mixture of hydrocarbons, mostly alkanes.

It can be separated at a fractionating column with a temperature gradient due to difference in boiling point. (Passes through a series of trays containing bubble caps and condense at different points)

Smaller chains: more demanded thus higher value, and ethene makes polyethene.



CRACKING

- Breaking C-C bonds in alkanes

Thermal cracking

- High temperature and high pressure (700-1200k) (7000kPa)
- High % of alkenes produced.

Catalytic cracking

- Lower temperature and lower pressure

(720k) (2atp)

- Zeolite/aluminosilicate catalyst
- High % of motor fuels and aromatic hydrocarbons

Combustion of Alkanes:

Complete: makes water and carbon dioxide

Incomplete: carbon monoxide, carbon, carbon dioxide and water.

CO – toxic: binds irreversibly to haemoglobin

Carbon: aggravates asthma and other respiratory illnesses.

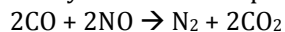
Carbon dioxide and water: greenhouse gas, contributes to global warming

INTERNAL COMBUSTION ENGINE POLLUTANTS:

NO_x – Nitrogen oxides → N₂ + O₂ → 2NO § High temp due to engine and sparks N₂ and O₂ in air reacts, forms Nitric acid and acid rain and photochemical smog.

Removal of pollutants:

Catalytic converters: palladium, platinum, or rhodium.



Hydrocarbon + Nitrogen oxide \rightarrow Nitrogen + Carbon dioxide + water

Sulphur dioxide \rightarrow (Sulphur impurities from crude oil)

When combusted, $\text{SO}_2 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_3$ which $+ \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{SO}_4$

REMOVAL: Flue gas desulphurization using Calcium oxide, forming CaSO_4

Greenhouse gases: Methane, water vapor and carbon dioxide.

High-energy radiation penetrates atmosphere and enters the earth, re-emitted at a lower frequency and longer wavelength. Some fails to pass through the blanket of greenhouse gases, stays in earth and heats it up.

Nomenclature (naming)

Family	Formula	Suffix	Example
alkanes	$\text{CH}_3(\text{CH}_2)_n\text{CH}_3$ R-H	-ane	ethane
alkenes	$\text{CH}_3(\text{CH}_2)_n\text{CH}=\text{CH}_2$ R-CH=CH ₂	-ene	propene
haloalkanes	$\text{CH}_3(\text{CH}_2)_n\text{CH}_2\text{X}$ (X = F, Cl, Br or I) R-X	none	chloromethane CH ₃ Cl
alcohols	$\text{CH}_3(\text{CH}_2)_n\text{CH}_2\text{OH}$ R-OH	-ol	ethanol C ₂ H ₅ OH
aldehydes	$\text{CH}_3(\text{CH}_2)_n\text{CHO}$ R-CHO	-al	ethanal CH ₃ CHO
ketones	$\text{CH}_3(\text{CH}_2)_n\text{CO}(\text{CH}_2)_n\text{CH}_3$ R-COR'	-one	propanone CH ₃ COCH ₃
carboxylic acids	$\text{CH}_3(\text{CH}_2)_n\text{COOH}$ R-COOH	-oic acid	ethanoic acid CH ₃ COOH

- smallest number for functional group
- Number in front of every branch

- Halogen first then branch
- Halogen arranged alphabetically