2.1 Atoms and reactions

2.1.1 Atomic structure and isotopes

- Definitions

Term	Definition
Isotopes	Atoms of the same element with the same number of **protons and electrons** and **different numbers of neutrons and different masses**.
Proton number / atomic number	The number of **protons** in the nucleus of an atom.
Nucleon number / mass number	The number of **protons and neutrons** in the nucleus of an atom.
Relative isotopic mass / A	The mass of an isotope of an element compared to 1/12th of the mass of an carbon-12 atom.
Relative atomic mass / A_r / A_R	The **weighted mean** mass of an atom of an element compared to 1/12 of the mass of an atom of carbon-12.
Cation	A **positively charged** ion with fewer electrons than protons.
Anion	A **negatively charged** ion with more electrons than protons.

- Properties of isotopes
  - Same chemical reactions
    - Same electron configuration & the same number of protons
    - Number of neutrons has no effect on reactions of an element
  - Small differences in physical properties
    - Higher mass isotopes = higher melting and boiling point + higher density
- Mass and charge of sub-atomic particles

Particle	Relative charge	Relative mass
Proton / p^+	1+	1
Neutron / n	0	1
Electron / e^-	1-	1/1836

- Determining relative atomic mass and relative isotopic mass (for ions with single charges)
  - Mass spectrometer
  - Records abundance of ions of different isotopes and their mass-to-charge ratio (m/z ratio)
  - Value of relative isotopic mass can be worked out from m/z ratio and hence relative atomic mass

2.1.2 Compounds, formulae and equations

- Definitions

Term	Definition
Binary compounds	Compounds that contains **two elements** only.
Diatomic molecules	Molecules composed of **two atoms** only.
Polyatomic ions	Ion containing more than one atoms.

- Anions to know

Ion	Formula
Nitrate	NO_3^-
Carbonate	CO_3^{2-}
Sulfate	SO_4^{2-}

Hydroxide	OH^-

- Cations to know
Ion	Formula
Ammonium	NH_4^+
Zinc ion	Zn^{2+}
Silver ion	Ag^+
- Writing ionic equations
    - We can only dissociate the **aqueous compounds**
    - Split all chemicals into ions
    - Cancel out spectator ions
    - No aqueous compound = no ionic equation
- Solubility
Solubility	Compounds
Soluble in water	• All common sodium, potassium and ammonium salts (also their carbonate and hydroxide salt) • All nitrates • Most common chlorides • Most common sulfates
Insoluble in water	• **Silver chloride, lead chloride** • **Lead sulfate, barium sulfate, calcium sulfate, strontium sulfate** • Most common carbonates • Most common hydroxides

2.1.3 Amount of substance

- Definitions
Term	Definition
Mole	A mole is the amount of a substance that contains the Avogadro number of elementary particles / the amount of a substance that contains the same amount of particles as 12 g of carbon-12.
Molar mass / M	The mass in grams in each mole of the substance, measured in g mol^{-1}.
Hydrated	A crystalline compound that contains water (e.g. $CuSO_4{\cdot}5H_2O_{(s)}$).
Anhydrous	A crystalline compound containing no water (e.g. $CuSO_{4(s)}$).
Water of crystallisation	Water molecules that form part of the crystalline structure of a compound (e.g. H_2O in $CuSO_4{\cdot}5H_2O_{(s)}$).
Stoichiometry	The relative quantities of substances in a reaction.
Standard solution	A solution of known concentration.
Limiting reagent	The reactant that is not in excess and will be used up in the reaction.
- Amount of substance
    - Symbol n
    - Measured in moles (symbol mol)
    - * Always use **decimals (not fractions)** in **every step** of a calculation
- Avogadro constant / N_A
    - $6.02\times10^{23}\ \mathrm{mol}^{-1}$
    - The number of particles per mole
- Concentration (c)
    - Unit = mol dm^{-3} (aka molar / M) or g dm^{-3}
    - mol dm^{-3}: $c = \frac{n}{V} = \frac{\text{number of moles}}{\text{volume (in dm}^{-3})}$

- g dm-3: $c = \frac{\text{mass (in g)}}{\text{volume (in dm}^{-3})}$
- $\text{Concentration in mol dm}^{-3} = \frac{\text{concentration in g dm}^{-3}}{M_r}$
- Room temperature and pressure (RTP)
  - Temp = 20 °C / 293 K
  - pressure = 1 atm or 1.01×10^5 Nm^{-2}
- Standard temperature and pressure (STP)
  - Temp = 0 °C / 273 K
  - pressure = 1 atm or 1.01×10^5 Nm^{-2}
- Molar gas volume / V_m
  - The volume per mole of gas at a stated temperature and pressure
  - Under RTP: 1 mol = 24 dm^3 = 24,000 cm^3
  - Under STP: 1 mol = 22.4 dm^3 = 22,400 cm^3
- Ideal gas equation
  - $pV = nRT$
  - $p =$ pressure (Pa or N m^{-2})
  - $V =$ volume (m^3)
  - $n =$ amount of gas molecules (mol)
  - $R =$ ideal gas constant (8.314 J mol^{-1} K^{-1})
  - $T =$ temperature (**K not °C**)
  - Rearranged: $\frac{p_1 v_1}{T_1} = \frac{p_2 v_2}{T_2}$
- Ideal gas assumptions
  - Random motion in straight lines
  - Molecules behave as rigid spheres
  - Pressure is due to collisions between the molecules and the walls of the container
  - Elastic collisions between the molecules and between the molecules and the walls of the container
  - Temperature of the gas ∝ average KE of the molecules
  - The molecules occupy an entirely negligible volume
  - No intermolecular forces between the gas molecules
- Percentages yield
  - $\text{Percentage yield} = \frac{\text{actual yield}}{\text{thereotical yield}} \times 100\%$
  - Actual yield: the amount of the product obtained from a reaction
  - Theoretical yield: the yield resulting from complete conversion of reactants into products
  - Reasons for < 100% percentage yield
    - Reaction did not go to completion
    - Side reactions may have taken place along the main reaction
    - Purification of the product may result in the loss of some products
- Atom economy
  - $\text{Atom economy} = \frac{\text{sum of masses of useful product(s)}}{\text{sum of masses of all products or reactants}} \times 100\%$
    $= \frac{\text{sum of molar masses of useful products}}{\text{sum of molar masses of all products or reactants}} \times 100\%$
- Benefits of high atom economy
  - More efficient industrial process
  - Preserve raw materials
  - Reduce waste
- Means to improve sustainability
  - Use processes with high atom economy and fewer steps
  - Redesign methods to use less hazardous starting materials
  - Use milder reaction conditions / better catalysts / less hazardous solvents
- Experimental techniques

Variable measured	Method

Mass	• Use a digital mass balance • Choose a balance with a suitable resolution for the experiment
Volume of solution	• Use a measuring cylinder • Standard solution: use volumetric flask
Gas produced	• Use a gas syringe / measure mass lost on a balance and calculate the number of moles of gas produced

- Types of formulae

Formula	**Meaning**
Empirical formula	The **simplest whole number ratio** of atoms of each element present in a compound.
Molecular formula	The number and type of atoms of each element in a molecule (**if the elements are the same then combine them, e.g. not CH_3COOH, use $C_2H_4O_2$**).
Displayed (graphical) formula	Shows all the bonds in the structure.
Structural formula	A molecular formula that shows not only what atoms are present but also how they are joined together.

2.1.4 Acids

- Acids
    - When dissolved in water an acid releases H^+ ions (proton) into the solution
    - Common acids
        - HCl
        - H_2SO_4
        - HNO_3
        - CH_3COOH
- Bases
    - React with acid by **accepting H^+ ions (protons)** and neutralising the acid to form a salt
    - Common bases
        - Carbonates
        - Hydrogencarbonates
        - Metal oxides
        - Metal hydroxides
        - Ammonia (accept H^+ and form $NH4^+$ ions)
- Alkalis
    - Bases that dissolve in water and release OH^- ions into the solution
    - Common alkalis
        - NaOH
        - KOH
        - NH_3
- Salt
    - When the H^+ in an acid is replaced by a positive ion
- Strong and weak acid
    - Both release H^+ ions / H^+ donor in aqueous solutions
    - Strong acid
        - **Completely dissociates** in aqueous solutions / releases all hydrogen atoms as H^+ ions
        - e.g. $HCl(aq) \rightarrow H^+(aq) + Cl^-(aq)$
    - Weak acid
        - **Partially dissociates** in aqueous solutions / only releases a portion of available hydrogen atoms as H^+ ions
        - e.g. $CH_3COOH(aq) \rightleftharpoons H^+(aq) + CH_3COO^-(aq)$
- Neutralisation
    - The reaction of acids with bases (including carbonates, metal oxides and alkalis) to form salts

- Ionic equation: $H^+(aq) + OH^-(aq) \rightarrow H_2O(l)$
- Preparing standard solution
  - Solid weighed accurately **using a balance with 2 dp or more**
  - Dissolve solid in a beaker
    - Use less distilled water than needed to fill the volumetric flask to the mark
  - Transfer the solution to (250 cm^3) volumetric flask
    - Rinse the beaker and transfer washings to the flask so the last traces of the solution is transferred to the volumetric flask
  - Volumetric flask is filled to the graduation line
    - Add distilled water a drop at a time using a dropping pipette
    - Keep adding until the bottom of the meniscus lines up exactly with the mark
  - Mix the solution thoroughly
    - Volumetric flask is sealed with a stopper and inverted several times
- Titration
  - Add measured volume of one solution to conical flask using pipette
    - Typical tolerances: 10 cm^3: ± 0.04 cm^3, 25 cm^3: ± 0.04 cm^3, 50 cm^3: ± 0.10 cm^3
  - Add other solution to burette, record initial reading
  - Add a few drops of indicator to conical flask (phenolphthalein / methyl orange)
  - Run solution from burette into conical flask until it reaches the end point
    - Swirl the flask while the solution is added
  - Record final reading
  - Titre = final reading - initial reading
  - First titre carried out quickly to get approximate titre
  - Repeat accurately by adding solution dropwise as the end point is approached
  - Carry out until two accurate titres are concordant (within 0.1 cm^3)
  - * Only use concordant results for calculating the mean titre

2.1.5 Redox

- Definitions

Term	Definition
Redox reactions	A reaction involving reduction and oxidation.
Oxidising agent	A reagent that **accepts / takes in** electrons.
Reducing agent	A reagent that **donates / gives out** electrons.
Oxidation number	A measure of the number of electrons that an atom uses to bond with atoms of another element. Oxidation numbers are derived from a set of rules.

- Oxidation number (oxidation state) rules
  - Elements
    - **Always 0**
    - Any bonding is to atoms of the same element in pure elements
  - Compound and ions
    - Each atom in a compound has an oxidation number
    - Sign is placed before the number
    - Sum of oxidation numbers in a compound / ion = total charge
- Fixed oxidation numbers

Combined element	Oxidation number
O (normally)	-2
H (normally)	+1
F	-1
Group 1	+1
Group 2	+2

Group 3	+3

- Oxidation number for special cases
Combined element	Oxidation number
H in metal hydrides (e.g. NaH, CaH_2)	-1
O in peroxide ions (O_2^{2-})	-1
O bonded to F (e.g. F_2O)	+2
- Roman numerals in chemical names
  - Show oxidation number without sign
  - Nitrate = assume to be NO_3^-
  - Sulfate = assume to be SO_4^{2-}
  - e.g. chlorate(I) = ClO^-
- Redox reaction
  - Oxidation
    - Gain of oxygen
    - Loss of hydrogen
    - Loss of electrons
    - Increase in oxidation number
  - Reduction
    - Loss of oxygen
    - Gain of hydrogen
    - Gain of electrons
    - Decrease in oxidation number

  * Oxidation and reduction always **happen together**
- Redox reaction of acids
  - Metal + acid → salt + hydrogen
  - Metal oxidised (oxidation number increases from 0 to …)
  - Hydrogen in acid reduced (oxidation number decreases from +1 to 0)
  - (Iron is normally Fe^{2+} in redox reactions)