Formulae, equations and amount of substance

Terms and formulae, the mole, relative masses, concentration, empirical and molecular formulae, reacting masses and gas volumes, yield and atom economy, and equations with state symbols.

Terms and formulae

- An **atom** is the smallest particle of an element that can take part in a chemical change.
- An **element** has atoms with the same atomic number.
- An **ion** is an atom or group of atoms with a charge.
- A **molecule** is a group of atoms joined by covalent bonds.
- A **compound** has two or more elements chemically combined in a fixed ratio.
- The **empirical formula** is the simplest whole-number ratio of atoms of each element in a compound.
- The **molecular formula** is the actual number of atoms of each element in one molecule.

> **NOTE**
>
> Ethane has molecular formula C_2H_6 and empirical formula CH_3. Giant structures such as sodium chloride have only an empirical formula, and the term **relative formula mass** is used for them.

Relative masses and the mole

Relative atomic mass A_r is the weighted mean mass of an atom of an element, compared with $\frac{1}{12}$ of the mass of an atom of carbon-12. **Relative molecular mass** M_r is the sum of the A_r values of the atoms in a molecule.

The **mole** is the unit of amount of substance. One mole contains the **Avogadro constant**, $L = 6.02 \times 10^{23}$ mol^{-1}, of particles. **Molar mass** is the mass of one mole, in g mol^{-1}.

$$n = \frac{m}{M} \qquad \text{number of particles} = n \times L$$

> **TRY IT**
>
> How many chloride ions are in 5.35 g of ammonium chloride, NH_4Cl ($M = 53.5$ g mol^{-1})?

$n = \dfrac{5.35}{53.5} = 0.100$ mol of NH_4Cl, so 0.100 mol of Cl^-. Number of ions $= 0.100 \times 6.02 \times 10^{23} = 6.02 \times 10^{22}$.

Note Academy

Parts per million

$$\text{ppm} = \frac{\text{mass (or volume) of the component}}{\text{total mass (or volume)}} \times 10^6$$

For gases in the atmosphere, ppm by volume is used. Air containing 0.04% carbon dioxide has $0.04 \times 10^4 = 400$ ppm.

Concentration

$c = \frac{n}{V}$ (mol dm^{-3}, V in dm^3) concentration in g dm^{-3} $= c \times M$

Convert cm^3 to dm^3 by dividing by 1000.

> **TRY IT**
>
> 2.00 g of sodium hydroxide is dissolved in water to make 250 cm^3 of solution. Find the concentration in mol dm^{-3} and g dm^{-3}.

$n = 2.00/40.0 = 0.0500$ mol. $c = 0.0500/0.250 = 0.200$ mol dm^{-3}, which is $0.200 \times 40.0 = 8.00$ g dm^{-3}.

Empirical and molecular formulae

1. Divide each mass (or percentage) by the A_r to get moles of each element.
2. Divide all by the smallest to get a ratio.
3. Multiply to clear any fractions (1.5 becomes 3 : 2, 1.33 becomes 4 : 3).
4. For the molecular formula, divide the molar mass by the empirical formula mass and multiply the empirical formula by this whole number.

> **TRY IT**
>
> A compound is 85.7% carbon and 14.3% hydrogen by mass and has $M_r = 56$. Find its molecular formula.

C: $85.7/12.0 = 7.14$. H: $14.3/1.0 = 14.3$. Ratio $1 : 2$, so the empirical formula is CH_2 (mass 14). $56/14 = 4$, so the molecular formula is C_4H_8.

Equations and reacting masses

A balanced equation gives the ratio of moles. Include **state symbols**: (s), (l), (g), (aq).

A **full** equation shows all the formulae. An **ionic** equation shows only the species that change, leaving out spectator ions.

$$Ba^{2+}(aq) + SO_4^{2-}(aq) \rightarrow BaSO_4(s)$$

Note Academy

To find a reacting mass: convert mass to moles, use the mole ratio from the equation, and convert moles back to mass.

> **TRY IT**
>
> What mass of carbon dioxide forms when 10.0 g of calcium carbonate is heated? $CaCO_3 \rightarrow CaO + CO_2$

$n(CaCO_3) = 10.0/100.1 = 0.0999$ mol. The ratio is 1 : 1, so $n(CO_2) = 0.0999$ mol and $m = 0.0999 \times 44.0 = 4.40$ g.

Volumes of gases

At room temperature and pressure (about 298 K and 100 kPa) one mole of any gas occupies about 24 dm^3. For other conditions use the **ideal gas equation**:

$$pV = nRT$$

with p in Pa, V in m^3, T in kelvin and $R = 8.31$ J K^{-1} mol^{-1}. The same equation gives the molar mass of a volatile liquid from its mass and the volume of vapour it produces.

> **TRY IT**
>
> 0.150 g of a volatile liquid forms 48.0 cm^3 of vapour at 100 kPa and 373 K. Find its molar mass.

$n = \dfrac{pV}{RT} = \dfrac{100000 \times 48.0 \times 10^{-6}}{8.31 \times 373} = 1.55 \times 10^{-3}$ mol. $M = 0.150/1.55 \times 10^{-3} = 96.8$ g mol^{-1}.

> **NOTE**
>
> Core Practical 1 measures the molar volume of a gas, for example by collecting carbon dioxide from marble chips and acid in a gas syringe, or hydrogen from magnesium and acid. Use the moles of the limiting reactant, and make sure the gas is not lost before the syringe is connected.

Percentage yield and atom economy

$$\text{percentage yield} = \frac{\text{actual mass (or moles) of product}}{\text{theoretical mass (or moles) of product}} \times 100$$

$$\text{atom economy} = \frac{M_r \text{ of the desired product}}{\text{sum of } M_r \text{ of all products}} \times 100\%$$

Yield tells you how much was made compared with the maximum. Atom economy tells you how much of the reactant mass ends up in the product you want. A reaction with a high yield can still have a low atom economy if it makes a lot of waste.

Note Academy

Industrial processes aim for high atom economy to reduce waste and use of resources.

Reactions in test tubes

Relate equations to observations.

- **Displacement.** A more reactive metal displaces a less reactive one: $Zn(s) + Cu^{2+}(aq) \rightarrow Zn^{2+}(aq) + Cu(s)$. Blue colour fades and brown copper forms.
- **Acids.** With metals they give a salt and hydrogen. With carbonates they give a salt, water and carbon dioxide (effervescence). With bases they give a salt and water.
- **Precipitation.** Mixing solutions can make an insoluble solid: $Ag^{+}(aq) + Cl^{-}(aq) \rightarrow AgCl(s)$, a white precipitate.

> **When you write an ionic equation, cancel spectator ions, check the charges balance as well as the atoms, and add state symbols.**

Note Academy