Formulae and the Mole

Chemical formulae and equations, relative atomic and molecular masses, the mole and the Avogadro constant, gas volumes, concentration, reacting masses, limiting reactants, titration calculations, empirical and molecular formulae, percentage yield and percentage purity.

NOTE

Relative atomic masses used in these notes: H 1, C 12, N 14, O 16, Na 23, Mg 24, Al 27, S 32, Cl 35.5, K 39, Ca 40, Fe 56, Cu 64, Zn 65, Ag 108. In the exam these are given in the Periodic Table.

3.1 Formulae

A **formula** uses chemical symbols and numbers to show the atoms in a substance. The small number after a symbol is the number of atoms of that element, for example H_2SO_4 has two hydrogen, one sulfur and four oxygen atoms.

Substance	Formula	Substance	Formula
water	H_2O	ammonia	NH_3
carbon dioxide	CO_2	methane	CH_4
hydrochloric acid	HCl	sodium hydroxide	$NaOH$
sulfuric acid	H_2SO_4	calcium carbonate	$CaCO_3$
nitric acid	HNO_3	sodium chloride	$NaCl$

The molecular formula shows the actual number and type of each atom in one molecule. The empirical formula is the simplest whole-number ratio of the atoms or ions in a compound.

Glucose has the molecular formula $C_6H_{12}O_6$ and the empirical formula CH_2O. Ethene is C_2H_4 and its empirical formula is CH_2. For ionic compounds and giant covalent substances such as $NaCl$ and SiO_2, the formula is always the empirical formula.

Formulae from a diagram. To deduce a formula from a model or diagram, count the atoms of each element in one unit. For example, a diagram of a molecule with one carbon atom bonded to four hydrogen atoms gives CH_4.

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The formula of an ionic compound

An ionic compound is neutral overall, so the **total positive charge equals the total negative charge**. Use the charges on the ions.

Positive ions	Negative ions
H^+, Li^+, Na^+, K^+, Ag^+, NH_4^+	Cl^-, Br^-, I^-, OH^-, NO_3^-
Mg^{2+}, Ca^{2+}, Ba^{2+}, Zn^{2+}, Cu^{2+}, Fe^{2+}, Pb^{2+}	O^{2-}, S^{2-}, CO_3^{2-}, SO_4^{2-}
Al^{3+}, Fe^{3+}, Cr^{3+}	N^{3-}, PO_4^{3-}

> **TRY IT**
>
> Deduce the formulae of (a) calcium chloride, (b) aluminium oxide, (c) ammonium sulfate.

(a) Ca^{2+} needs two Cl^- to balance: $CaCl_2$. (b) Al^{3+} and O^{2-}: the lowest common multiple of 3 and 2 is 6, so two Al^{3+} $(+6)$ and three O^{2-} (-6): Al_2O_3. (c) NH_4^+ and SO_4^{2-}: two NH_4^+ are needed, and brackets are used around a group of atoms: $(NH_4)_2SO_4$.

A Roman numeral in a name gives the charge on a metal ion: iron(III) oxide contains Fe^{3+} and O^{2-}, so its formula is Fe_2O_3.

Equations

A **word equation** uses names. A **symbol equation** uses formulae and must be **balanced**: the same number of each type of atom on both sides. Never change a formula to balance an equation; change the **numbers in front**.

State symbols: (s) solid, (l) liquid, (g) gas, (aq) dissolved in water.

$$\text{magnesium} + \text{oxygen} \rightarrow \text{magnesium oxide}$$

$$2\,Mg\,(s) + O_2\,(g) \longrightarrow 2\,MgO\,(s)$$

> **TRY IT**
>
> Balance: $Al + Cl_2 \longrightarrow AlCl_3$ and $C_3H_8 + O_2 \longrightarrow CO_2 + H_2O$.

$$2\,Al\,(s) + 3\,Cl_2\,(g) \longrightarrow 2\,AlCl_3\,(s)$$

$$C_3H_8\,(g) + 5\,O_2\,(g) \longrightarrow 3\,CO_2\,(g) + 4\,H_2O\,(l)$$

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Ionic equations

An **ionic equation** shows only the ions (and substances) that actually take part in the reaction. The ions that are unchanged, called **spectator ions**, are left out. Both the atoms and the **charges** must balance.

For silver nitrate and sodium chloride solutions, a white precipitate of silver chloride forms:

$$\mathrm{AgNO_3(aq) + NaCl(aq) \longrightarrow AgCl(s) + NaNO_3(aq)}$$

The $\mathrm{Na^+}$ and $\mathrm{NO_3^-}$ ions are spectators, so the ionic equation is:

$$\mathrm{Ag^+(aq) + Cl^-(aq) \longrightarrow AgCl(s)}$$

To write an ionic equation: write the balanced symbol equation with state symbols, split everything that is $\mathrm{(aq)}$ and ionic into ions, cancel the ions that are the same on both sides, and write what remains.

3.2 Relative masses of atoms and molecules

The relative atomic mass, A_r, is the average mass of the isotopes of an element, compared with $\frac{1}{12}$ of the mass of an atom of carbon-12. The relative molecular mass, M_r, is the sum of the relative atomic masses of all the atoms in the formula. For ionic compounds it is called the relative formula mass.

A_r and M_r have **no units**.

TRY IT

Calculate the M_r of (a) $\mathrm{H_2SO_4}$, (b) $\mathrm{Ca(OH)_2}$, (c) $\mathrm{CuSO_4 \cdot 5\,H_2O}$.

(a) $(2 \times 1) + 32 + (4 \times 16) = 2 + 32 + 64 = 98$. (b) $40 + 2 \times (16 + 1) = 40 + 34 = 74$. (c) $\mathrm{CuSO_4}$ is $64 + 32 + 64 = 160$ and $5\ \mathrm{H_2O}$ is $5 \times 18 = 90$, so $160 + 90 = 250$.

3.3 The mole and the Avogadro constant

The mole (symbol mol) is the unit for the amount of substance. One mole contains 6.02×10^{23} particles (atoms, ions or molecules). This number is the Avogadro constant.

The **molar mass** is the mass of one mole, in $\mathrm{g/mol}$. It has the same number as the A_r or M_r. So one mole of carbon is $12\ \mathrm{g}$ and one mole of $\mathrm{CO_2}$ is $44\ \mathrm{g}$.

$$\text{amount of substance (mol)} = \frac{\text{mass (g)}}{\text{molar mass (g/mol)}} \qquad n = \frac{m}{M}$$

$$\text{number of particles} = n \times 6.02 \times 10^{23}$$

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(a) Find the mass of 0.25 mol of $CaCO_3$. (b) How many moles are in 4.0 g of $NaOH$? (c) How many molecules are in 0.50 mol of H_2O?

(a) $M_r = 40 + 12 + 48 = 100$, so $m = 0.25 \times 100 = 25$ g. (b) $M_r = 23 + 16 + 1 = 40$, so $n = \frac{4.0}{40} = 0.10$ mol. (c) $0.50 \times 6.02 \times 10^{23} = 3.01 \times 10^{23}$ molecules.

Gases

One mole of any gas occupies 24 dm^3 at room temperature and pressure (r.t.p.).

$$\text{volume of gas (dm}^3\text{)} = n \times 24 \qquad \text{or} \qquad n = \frac{\text{volume in dm}^3}{24} = \frac{\text{volume in cm}^3}{24\,000}$$

1 dm^3 $= 1000$ cm^3, so **divide by** 1000 to change cm^3 into dm^3.

Concentration

The **concentration** of a solution is the amount of solute in 1 dm^3 of solution, in either g/dm^3 or mol/dm^3.

$$\text{concentration (g/dm}^3\text{)} = \frac{\text{mass (g)}}{\text{volume (dm}^3\text{)}} \qquad \text{concentration (mol/dm}^3\text{)} = \frac{n}{\text{volume (dm}^3\text{)}}$$

$$\text{concentration in mol/dm}^3 = \frac{\text{concentration in g/dm}^3}{M_r} \qquad n = \text{concentration} \times \text{volume in dm}^3$$

TRY IT

5.0 g of sodium hydroxide is dissolved in water to make 250 cm^3 of solution. Find the concentration in g/dm^3 and in mol/dm^3.

Volume $= 250 \div 1000 = 0.250$ dm^3. In g/dm^3: $\frac{5.0}{0.250} = 20$ g/dm^3. In mol/dm^3: $\frac{20}{40} = 0.50$ mol/dm^3.

Reacting masses and gas volumes

The **balanced equation** gives the ratio of moles. The method:

1. Write the balanced equation.
2. Work out the moles of the substance you are given ($n = m \div M_r$, or from volume or concentration).
3. Use the **mole ratio** from the equation to find the moles of the substance you want.

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4. Convert to a mass, a volume of gas, or a concentration.

> **TRY IT**
>
> Calculate the mass of calcium oxide made by heating $10\ \text{g}$ of calcium carbonate: $\text{CaCO}_3 \longrightarrow \text{CaO} + \text{CO}_2$.

$n(\text{CaCO}_3) = \dfrac{10}{100} = 0.10\ \text{mol}$. The ratio is $1 : 1$, so $n(\text{CaO}) = 0.10\ \text{mol}$. $M_\text{r}(\text{CaO}) = 56$, so mass $= 0.10 \times 56 = 5.6\ \text{g}$.

> **TRY IT**
>
> $\text{Mg} + 2\,\text{HCl} \longrightarrow \text{MgCl}_2 + \text{H}_2$. What mass of magnesium gives $120\ \text{cm}^3$ of hydrogen at r.t.p.?

$n(\text{H}_2) = \dfrac{120}{24\,000} = 0.0050\ \text{mol}$. The ratio $\text{Mg} : \text{H}_2$ is $1 : 1$, so $n(\text{Mg}) = 0.0050\ \text{mol}$ and the mass is $0.0050 \times 24 = 0.12\ \text{g}$.

Limiting reactants

The **limiting reactant** is the one that is used up first, and it decides how much product forms. The other reactant is **in excess**. To find it, work out the moles of each reactant and compare with the equation.

> **TRY IT**
>
> $2.4\ \text{g}$ of magnesium is added to $100\ \text{cm}^3$ of $1.0\ \text{mol/dm}^3$ hydrochloric acid: $\text{Mg} + 2\,\text{HCl} \longrightarrow \text{MgCl}_2 + \text{H}_2$. Which is limiting, and what volume of hydrogen forms at r.t.p.?

$n(\text{Mg}) = \dfrac{2.4}{24} = 0.10\ \text{mol}$ and $n(\text{HCl}) = 1.0 \times 0.100 = 0.10\ \text{mol}$. The equation needs 2 mol of HCl for every 1 mol of Mg, so $0.10\ \text{mol}$ of Mg needs $0.20\ \text{mol}$ of HCl. The **acid is limiting**. $n(\text{H}_2) = 0.10 \div 2 = 0.050\ \text{mol}$, so the volume is $0.050 \times 24 = 1.2\ \text{dm}^3$.

Titration calculations

In a titration, the volumes of two solutions that react exactly are measured, and the concentration of one is found from the other.

> **TRY IT**
>
> $25.0\ \text{cm}^3$ of sodium hydroxide solution is exactly neutralised by $20.0\ \text{cm}^3$ of $0.100\ \text{mol/dm}^3$ hydrochloric acid: $\text{NaOH} + \text{HCl} \longrightarrow \text{NaCl} + \text{H}_2\text{O}$. Find the concentration of the sodium

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hydroxide.

$n(\text{HCl}) = 0.100 \times \dfrac{20.0}{1000} = 0.00200$ mol. The ratio is $1:1$, so $n(\text{NaOH}) = 0.00200$ mol.

Concentration $= \dfrac{0.00200}{0.0250} = 0.0800$ mol/dm^3.

Empirical and molecular formulae

To find the empirical formula from masses or percentages: **divide each by its A_r** to get moles, then **divide by the smallest** to get the simplest whole-number ratio.

TRY IT

A compound is 85.7% carbon and 14.3% hydrogen by mass, and its M_r is 56. Find its empirical and molecular formulae.

Carbon: $\dfrac{85.7}{12} = 7.14$. Hydrogen: $\dfrac{14.3}{1} = 14.3$. Dividing by 7.14 gives the ratio $1:2$, so the empirical formula is CH_2 (mass 14). $\dfrac{56}{14} = 4$, so the molecular formula is C_4H_8.

TRY IT

4.8 g of magnesium combines with 3.2 g of oxygen. Find the empirical formula.

Mg: $\dfrac{4.8}{24} = 0.20$. O: $\dfrac{3.2}{16} = 0.20$. The ratio is $1:1$, so the formula is MgO.

Percentage yield, composition and purity

$$\text{percentage yield} = \frac{\text{actual mass obtained}}{\text{maximum (theoretical) mass}} \times 100$$

$$\text{percentage composition by mass of an element} = \frac{\text{mass of the element in one mole of the compound}}{M_r} \times 100$$

$$\text{percentage purity} = \frac{\text{mass of pure substance}}{\text{mass of the impure sample}} \times 100$$

TRY IT

(a) 10.0 g of CaCO_3 should give 5.6 g of CaO, but only 4.2 g is obtained. Find the percentage yield. (b) Find the percentage of nitrogen in ammonium nitrate, NH_4NO_3. (c) A 2.0 g sample of impure CaCO_3 gives 0.36 dm^3 of CO_2 at r.t.p. when heated. Find the percentage purity.

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(a) $\frac{4.2}{5.6} \times 100 = 75\%$. (b) $M_r = 14 + 4 + 14 + 48 = 80$, and there are 2 nitrogen atoms (28), so $\frac{28}{80} \times 100 = 35\%$. (c) $n(CO_2) = \frac{0.36}{24} = 0.015\ \text{mol}$, so $n(CaCO_3) = 0.015\ \text{mol}$ and its mass is $0.015 \times 100 = 1.5\ \text{g}$. Purity $= \frac{1.5}{2.0} \times 100 = 75\%$.

NOTE

Reasons the percentage yield is less than 100%: the reaction is reversible and does not go to completion, some product is lost when it is separated and transferred, or side reactions happen.

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