Formulae, Equations and Amount of Substance

Topic 1 of Unit 1 - Edexcel International A-Level Chemistry

Basic Chemical Concepts

Atom

The smallest unit of an element that retains its chemical properties.

Example: A single hydrogen atom (H)

> ### Analogy
> Atoms are like individual LEGO bricks - the basic building blocks of everything.

Element

A pure substance consisting of only one type of atom.

Example: Oxygen (O), Carbon (C), Iron (Fe)

> ### Analogy
> Elements are like different colors of LEGO bricks - each type is unique.

Ion

An atom or molecule that has gained or lost electrons, giving it a charge.

Example: Sodium ion (Na^+), Chloride ion (Cl^-)

> ### Analogy
> Ions are like LEGO bricks with extra pieces attached or missing pieces.

Molecule

Two or more atoms chemically bonded together.

Example: Water molecule (H_2O), Carbon dioxide (CO_2)

> ### Analogy
> Molecules are like small LEGO structures made by connecting individual bricks.

Compound

A substance formed when two or more different elements chemically combine.

Example: Water (H_2O), Sodium chloride (NaCl)

> ### Analogy
> Compounds are like complex LEGO models made from different colored bricks.

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Empirical vs Molecular Formulae

Empirical Formula

The simplest whole-number ratio of atoms in a compound.

> ### Example: Glucose
> Molecular formula: $C_6H_{12}O_6$
>
> Empirical formula: CH_2O (divided by 6)

> ### Example: Benzene
> Molecular formula: C_6H_6
>
> Empirical formula: CH (divided by 6)

Molecular Formula

The actual number of atoms of each element in a molecule.

> ### Example: Hydrogen Peroxide
>
> Molecular formula: **H_2O_2**
>
> Empirical formula: **HO** (divided by 2)

> ### Example: Ethane
>
> Molecular formula: **C_2H_6**
>
> Empirical formula: **CH_3** (divided by 2)

Finding Empirical Formula from Percentages

> ### Example: Compound with 40% C, 6.7% H, 53.3% O
>
> 1. Convert to moles: C: 40/12 = 3.33, H: 6.7/1 = 6.7, O: 53.3/16 = 3.33
> 2. Divide by smallest: C: 3.33/3.33 = 1, H: 6.7/3.33 = 2, O: 3.33/3.33 = 1
> 3. Empirical formula: **CH_2O**

> ### Analogy: Recipe vs. Actual Dish
>
> The empirical formula is like a basic recipe ratio (e.g., 1 part flour : 2 parts water), while the molecular formula is like the actual quantities used (e.g., 200g flour : 400g water). Both describe the same relationship, but one is simplified.

The Mole Concept and Avogadro's Constant

What is a Mole?

A **mole** is the SI unit for the amount of substance. It contains exactly **6.02×10^{23}** particles.

Just as:

- 1 dozen = 12 items
- 1 gross = 144 items
- 1 mole = 6.02×10^{23} particles

Avogadro's Constant

Named after Amedeo Avogadro, **Avogadro's constant (L)** is:

$$L = 6.02 \times 10^{23}\ \text{mol}^{-1}$$

This number was chosen so that 1 mole of carbon-12 atoms has a mass of exactly 12 grams.

Mole Calculations

Example: Converting mass to moles

Calculate the number of moles in 36g of water (H_2O)

1. Find molar mass of H_2O: $(2 \times 1) + 16 = 18$ g/mol
2. Apply formula: $n = m \div M$
3. Calculate: $n = 36\text{g} \div 18\ \text{g/mol} = 2\ \text{mol}$

Example: Converting moles to particles

Calculate the number of molecules in 3 moles of CO_2

1. Apply formula: $N = n \times L$
2. Calculate: $N = 3\ \text{mol} \times 6.02 \times 10^{23}\ \text{mol}^{-1}$

3. `Result: N = 1.806 × 10²⁴ molecules`

Analogy: The Mole as a Counting Unit

Imagine you're counting grains of sand on a beach. Counting them one by one would take forever! Instead, you could use a container that holds exactly 6.02×10^{23} grains of sand. This container is your "mole" of sand. Chemists use the same concept for atoms and molecules, which are too small to count individually.

Calculations Using the Mole Concept

Σ Key Formulas

Number of moles = Mass ÷ Molar Mass

$n = m \div M$

Number of particles = Moles × Avogadro's Constant

$N = n \times L$ (where $L = 6.02 \times 10^{23}\ mol^{-1}$)

Mass = Moles × Molar Mass

$m = n \times M$

Worked Examples

Example 1: Mass to Moles

Calculate the number of moles in 58.5g of NaCl

1. Find molar mass of NaCl: 23 + 35.5 = 58.5 g/mol
2. Apply formula: $n = m \div M$
3. Calculate: $n = 58.5g \div 58.5\ g/mol = 1.0\ mol$

Example 2: Moles to Particles

Calculate the number of molecules in 0.5 moles of CO_2

1. Apply formula: $N = n \times L$
2. Calculate: $N = 0.5\ mol \times 6.02 \times 10^{23}\ mol^{-1}$
3. Result: $N = 3.01 \times 10^{23}$ molecules

Example 3: Moles to Mass

Calculate the mass of 2.5 moles of H_2O

1. Find molar mass of H_2O: $(2 \times 1) + 16 = 18$ g/mol
2. Apply formula: $m = n \times M$
3. Calculate: $m = 2.5\ mol \times 18\ g/mol = 45g$

Common Pitfalls to Avoid

- Always check **units** - mass in grams, volume in dm^3, concentration in mol/dm^3
- Remember to **balance equations** before doing mole calculations
- For gases, use **molar volume** (24 dm^3 at room temperature) when needed
- When converting between units, use **scientific notation** for very large or small numbers

Writing Chemical Equations and State Symbols

Chemical Equations

A chemical equation represents a chemical reaction using **chemical formulas** and **symbols**.

Key components:

- **Reactants** - substances that react (left side)
- **Products** - substances formed (right side)
- **Arrow** (→) - indicates direction of reaction
- **Coefficients** - numbers before formulas showing ratios

State Symbols

State symbols indicate the physical state of each substance in the reaction:

Symbol	State	Example
(s)	Solid	$NaCl^{(s)}$
(l)	Liquid	$H_2O^{(l)}$
(g)	Gas	$O_2^{(g)}$
(aq)	Aqueous (dissolved in water)	$NaCl^{(aq)}$

Writing Chemical Equations

Example 1: Combustion of Methane

Methane (CH_4) reacts with oxygen to produce carbon dioxide and water

$$CH_4{}^{(g)} + 2O_2{}^{(g)} \rightarrow CO_2{}^{(g)} + 2H_2O^{(l)}$$

Example 2: Reaction of Sodium with Water

Sodium metal reacts with water to form sodium hydroxide and hydrogen gas

$$2Na^{(s)} + 2H_2O^{(l)} \rightarrow 2NaOH^{(aq)} + H_2{}^{(g)}$$

Example 3: Precipitation Reaction

Silver nitrate reacts with sodium chloride to form silver chloride precipitate

$$AgNO_3{}^{(aq)} + NaCl^{(aq)} \rightarrow AgCl^{(s)} + NaNO_3{}^{(aq)}$$

Analogy: Chemical Equations as Recipes

Think of a chemical equation like a recipe. The reactants are your ingredients, the products are what you make, and the coefficients tell you how much of each ingredient to use. State symbols are like notes on whether an ingredient is solid, liquid, gas, or dissolved in water (like salt in soup).

Balancing Chemical Equations

Conservation of Mass Principle

Law of Conservation of Mass

Mass cannot be created or destroyed in a chemical reaction. This means the **total mass of reactants** must equal the **total mass of products**.

To balance an equation, we ensure that the **same number of each type of atom** appears on both sides of the equation.

Step-by-Step Method

Balancing Process

1. Write the unbalanced equation with correct formulas
2. Count atoms of each element on both sides
3. Add coefficients (numbers in front) to balance
4. Check: count atoms again to verify balance
5. Reduce coefficients to smallest whole numbers

Worked Examples

Example 1: Hydrogen + Oxygen ⟶ Water

Unbalanced: $H_2 + O_2 \longrightarrow H_2O$

$$2H_2{}^{(g)} + O_2{}^{(g)} \rightarrow 2H_2O^{(l)}$$

Explanation: Added coefficient 2 to H_2 and H_2O to balance hydrogen atoms

Example 2: Methane + Oxygen ⟶ Carbon Dioxide + Water

Unbalanced: $CH_4 + O_2 \longrightarrow CO_2 + H_2O$

$$CH_4{}^{(g)} + 2O_2{}^{(g)} \rightarrow CO_2{}^{(g)} + 2H_2O^{(l)}$$

Explanation: Added coefficient 2 to O_2 and H_2O to balance oxygen and hydrogen atoms

Common Mistakes to Avoid

- Never change **subscripts** in formulas (changes the compound)
- Balance **polyatomic ions** as a unit when they appear on both sides

- Balance **hydrogen and oxygen** last (they often appear in multiple compounds)
- Always check your work by recounting atoms after balancing

Ionic Equations

What are Ionic Equations?

Ionic equations show **only the species that actually change** during a chemical reaction, omitting **spectator ions** that remain unchanged.

Key Features

- Show dissolved substances as separate ions
- Focus on the actual chemical change
- Useful for precipitation and redox reactions

Converting to Ionic Equations

Step-by-Step Process

1. Write the balanced full equation with state symbols
2. Split aqueous compounds into their ions
3. Identify and cancel spectator ions
4. Write the final ionic equation

Worked Example

Silver Nitrate + Sodium Chloride

Full equation:

$$AgNO_3{}^{(aq)} + NaCl^{(aq)} \rightarrow AgCl^{(s)} + NaNO_3{}^{(aq)}$$

Split into ions:

$$Ag^{+}(aq) + NO_3^{-}(aq) + Na^{+}(aq) + Cl^{-}(aq) \rightarrow AgCl(s) + Na^{+}(aq) + NO_3^{-}(aq)$$

Cancel spectator ions (Na^+ and NO_3^-):

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

This is the **ionic equation** showing only the ions that form the precipitate.

When to Use Ionic Equations

- **Precipitation reactions** - to identify which ions form the precipitate
- **Redox reactions** - to focus on electron transfer
- **Acid-base reactions** - to show proton transfer
- Never use for reactions involving **solids, liquids, or gases** as reactants or products

Relative Atomic Mass and the Carbon-12 Scale

What is Relative Atomic Mass?

The **relative atomic mass (Ar)** of an element is the average mass of its atoms compared to 1/12 of the mass of a carbon-12 atom.

Key Points

- Relative atomic mass has **no units** (it's a ratio)
- It accounts for all naturally occurring **isotopes** of an element
- Carbon-12 is the standard reference point

The Carbon-12 Scale

The carbon-12 scale defines the mass of a carbon-12 atom as exactly **12 atomic mass units (amu)**.

All other atomic masses are measured relative to this standard.

Example: Chlorine

Chlorine has two main isotopes:

Isotope	Mass (amu)	Abundance (%)
^{35}Cl	34.969	75.77%
^{37}Cl	36.966	24.23%

```
Ar(Cl) = (34.969 × 0.7577) + (36.966 × 0.2423)
Ar(Cl) = 26.49 + 8.96 = 35.45
```

Calculating Relative Atomic Mass

To calculate the relative atomic mass of an element:

```
Ar = Σ (isotope mass × fractional abundance)
```

Example: Magnesium

Magnesium has three isotopes:

- ^{24}Mg: 78.99% abundance, mass = 23.985 amu
- ^{25}Mg: 10.00% abundance, mass = 24.986 amu
- ^{26}Mg: 11.01% abundance, mass = 25.983 amu

```
Ar(Mg) = (23.985 × 0.7899) + (24.986 × 0.1000) +
(25.983 × 0.1101)
Ar(Mg) = 18.95 + 2.50 + 2.87 = 24.32
```

Analogy: Class Average Height

> Think of relative atomic mass like calculating the average height of students in a class. If 70% of students are 160cm tall and 30% are 170cm tall, the average height would be (160 × 0.7) + (170 × 0.3) = 163cm. Similarly, relative atomic mass is the weighted average of all isotope masses based on their natural abundance.

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Relative Molecular Mass and Relative Formula Mass

Key Differences

Relative Molecular Mass (Mr)

- Used for **discrete molecules**
- Sum of atomic masses of all atoms in a molecule
- Examples: H_2O, CO_2, CH_4

Relative Formula Mass (Mr)

- Used for **ionic compounds** with giant structures
- Sum of atomic masses in the formula unit
- Examples: NaCl, $CaCO_3$, Al_2O_3

Calculating Relative Molecular Mass

Example: Carbon Dioxide (CO_2)

Ar(C) = 12.0, Ar(O) = 16.0

```
Mr(CO₂) = Ar(C) + 2 × Ar(O)
Mr(CO₂) = 12.0 + 2 × 16.0
Mr(CO₂) = 44.0
```

Example: Glucose ($C_6H_{12}O_6$)

Ar(C) = 12.0, Ar(H) = 1.0, Ar(O) = 16.0

```
Mr(C₆H₁₂O₆) = 6 × Ar(C) + 12 × Ar(H) + 6 × Ar(O)
Mr(C₆H₁₂O₆) = 6 × 12.0 + 12 × 1.0 + 6 × 16.0
```

```
Mr(C₆H₁₂O₆) = 72.0 + 12.0 + 96.0 = 180.0
```

Σ Calculating Relative Formula Mass

Example: Sodium Chloride (NaCl)

Ar(Na) = 23.0, Ar(Cl) = 35.5

```
Mr(NaCl) = Ar(Na) + Ar(Cl)
Mr(NaCl) = 23.0 + 35.5 = 58.5
```

Example: Calcium Carbonate ($CaCO_3$)

Ar(Ca) = 40.0, Ar(C) = 12.0, Ar(O) = 16.0

```
Mr(CaCO₃) = Ar(Ca) + Ar(C) + 3 × Ar(O)
Mr(CaCO₃) = 40.0 + 12.0 + 3 × 16.0
Mr(CaCO₃) = 40.0 + 12.0 + 48.0 = 100.0
```

Key Point

Both relative molecular mass and relative formula mass are calculated the same way - by adding up the relative atomic masses of all atoms in the formula. The difference is in **when to use each term** based on the type of compound.

Molar Mass Calculations

What is Molar Mass?

Molar mass (M) is the mass of one mole of a substance, expressed in grams per mole (g/mol).

> ### Molar Mass = Relative Atomic/Molecular/Formula Mass (g/mol)
> The numerical value is the same, but the units are different!

For elements: M = Ar (g/mol)

For compounds: M = Mr (g/mol)

Calculating Molar Mass

> ### Example 1: Element (Sodium)
> Ar(Na) = 23.0
>
> ```
> M(Na) = 23.0 g/mol
> ```

> ### Example 2: Molecular Compound (Water)
> Mr(H_2O) = 18.0
>
> ```
> M(H₂O) = 18.0 g/mol
> ```

> ### Example 3: Ionic Compound (Sodium Chloride)
> Mr(NaCl) = 58.5
>
> ```
> M(NaCl) = 58.5 g/mol
> ```

Using Molar Mass in Calculations

> ### Example: Converting Mass to Moles
> Calculate the number of moles in 117g of NaCl
>
> 1. Find molar mass: M(NaCl) = 58.5 g/mol
> 2. Apply formula: n = m ÷ M

3. Calculate: $n = 117g \div 58.5$ g/mol = 2.0 mol

Example: Converting Moles to Mass

Calculate the mass of 0.5 moles of CO_2

1. Find molar mass: $M(CO_2) = 44.0$ g/mol
2. Apply formula: $m = n \times M$
3. Calculate: $m = 0.5$ mol $\times$ 44.0 g/mol = 22.0g

Common Mistakes to Avoid

- Always include **units** (g/mol) when stating molar mass
- Remember that **molar mass = relative mass** numerically, but with different units
- For polyatomic ions, calculate the molar mass of the **entire ion**
- Be careful with **significant figures** - use the same number as in the given data

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Parts per Million (ppm) Concept

What is ppm?

Parts per million (ppm) is a unit of concentration that represents one part of a substance per million parts of the total mixture.

Key Points

- 1 ppm = 1 mg of substance per kg of solution
- 1 ppm = 1 mg of substance per L of water (approximately)
- Used for **very dilute solutions** where percentage would be too small
- Common in environmental chemistry and air quality measurements

Calculating ppm

```
ppm = (mass of solute ÷ mass of solution) × 10⁶
```

Example: Water Contamination

A 2.0 kg water sample contains 0.004 g of lead. What is the concentration in ppm?

```
Mass of lead = 0.004 g = 0.004 g ÷ 1000 =
0.000004 kg
ppm = (0.000004 kg ÷ 2.0 kg) × 10⁶
ppm = 2 ppm
```

ppm in Atmospheric Chemistry

For gases, ppm is often expressed by **volume** rather than mass:

```
ppm (by volume) = (volume of gas ÷ total volume) ×
10⁶
```

Example: Carbon Dioxide in Atmosphere

Current atmospheric CO_2 levels are approximately 415 ppm by volume.

This means that in every 1,000,000 volume units of air, 415 units are CO_2.

Percentage = 415 ÷ 1,000,000 × 100% = 0.0415%

Analogy: Sugar in Swimming Pool

Imagine adding 1 gram of sugar to an Olympic-sized swimming pool (2.5 million liters of water). This would be approximately 0.4 ppm - a concentration so small you wouldn't taste it, but it would still be measurable with sensitive instruments. This helps illustrate how tiny concentrations can be significant in chemistry.

Concentration Calculations

What is Concentration?

Concentration is the amount of solute dissolved in a given volume of solvent.

Molar Concentration

- Measured in **mol dm^{-3}**
- Also called **molarity**
- Number of moles per cubic decimeter

Mass Concentration

- Measured in **g dm^{-3}**
- Mass of solute per cubic decimeter
- Common in industrial applications

Concentration Formulas

Molar Concentration (mol dm^{-3}) = moles of solute ÷ volume of solution (dm^3)

$c = n \div V$

Mass Concentration (g dm^{-3}) = mass of solute (g) ÷ volume of solution (dm^3)

$c = m \div V$

Note: 1 dm^3 = 1000 cm^3 = 1 liter

Worked Examples

Example 1: Calculating Molar Concentration

Calculate the concentration of a solution containing 0.5 moles of NaCl dissolved in 250 cm^3 of water.

1. Convert volume to dm^3: 250 cm^3 = 0.250 dm^3
2. Apply formula: $c = n \div V$

3. Calculate: $c = 0.5 \text{ mol} \div 0.250 \text{ dm}^3 = 2.0 \text{ mol dm}^{-3}$

Example 2: Converting Between Units

Convert a 1.5 mol dm^{-3} solution of HCl to g dm^{-3}. (Molar mass of HCl = 36.5 g/mol)

1. Find mass of 1 mole: 1 mol HCl = 36.5 g
2. Calculate mass concentration: $1.5 \text{ mol dm}^{-3} \times 36.5 \text{ g/mol} = 54.75 \text{ g dm}^{-3}$

Key Points to Remember

- Always check **units** - convert to dm^3 before calculating
- For dilute solutions, the volume of solute is often **negligible** compared to solvent
- To convert between mol dm^{-3} and g dm^{-3}, use the **molar mass**
- When preparing solutions, add solute to solvent, not the other way around

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Determining Empirical Formulae from Experimental Data

What is an Empirical Formula?

The **empirical formula** shows the simplest whole-number ratio of atoms in a compound.

Experimental data (mass or percentage composition) can be used to determine this formula.

Step-by-Step Method

From Mass Data

1. Convert masses to **moles** using molar masses
2. Divide all mole values by the **smallest** mole value
3. If needed, multiply all values to get **whole numbers**
4. Write the empirical formula using these ratios

Worked Example

Example: Compound with 2.4g of Carbon and 0.6g of Hydrogen

1. Convert to moles:
C: 2.4g ÷ 12g/mol = 0.20 mol
H: 0.6g ÷ 1g/mol = 0.60 mol

2. Divide by smallest (0.20):
C: 0.20 ÷ 0.20 = 1
H: 0.60 ÷ 0.20 = 3

3. Empirical formula: **CH_3**

Example: Compound with 40% C, 6.7% H, 53.3% O

1. Convert to moles (assume 100g total):
C: 40g ÷ 12g/mol = 3.33 mol
H: 6.7g ÷ 1g/mol = 6.7 mol
O: 53.3g ÷ 16g/mol = 3.33 mol

2. Divide by smallest (3.33):
C: 3.33 ÷ 3.33 = 1
H: 6.7 ÷ 3.33 = 2
O: 3.33 ÷ 3.33 = 1

3. Empirical formula: CH_2O

Common Pitfalls to Avoid

- Always use **accurate atomic masses** for calculations
- When values are close to whole numbers (e.g., 1.98), they can be **rounded**
- If you get values like 0.5, 1.5, or 2.5, **multiply all values** by 2
- For values like 0.33 or 0.67, **multiply all values** by 3
- Remember that empirical formula shows **ratios**, not actual numbers of atoms

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Determining Molecular Formulae from Empirical Formulae

Empirical vs Molecular Formula

Empirical Formula

- Simplest **ratio** of atoms
- May not represent actual molecule
- Example: CH_2O (for glucose)

Molecular Formula

- **Actual** number of atoms
- Multiple of empirical formula
- Example: $C_6H_{12}O_6$ (for glucose)

Step-by-Step Method

Finding Molecular Formula

1. Calculate the **relative molecular mass** of the empirical formula
2. Divide the **actual molecular mass** by the empirical formula mass
3. This gives the **multiplier** (n)
4. Multiply each subscript in the empirical formula by n

Worked Examples

Example 1: Compound with Empirical Formula CH_2O and Mr = 180

1. Mr of empirical formula: 12 + (2 × 1) + 16 = 30
2. Multiplier: 180 ÷ 30 = 6
3. Molecular formula: $C_6H_{12}O_6$

Example 2: Compound with Empirical Formula C_2H_5 and Mr = 58

1. Mr of empirical formula: (2 × 12) + (5 × 1) = 29
2. Multiplier: 58 ÷ 29 = 2
3. Molecular formula: C_4H_{10}

Key Points to Remember

- The molecular formula is always a **whole number multiple** of the empirical formula
- If the multiplier is 1, the empirical and molecular formulas are **identical**
- For compounds with **giant structures** (like NaCl), the empirical formula is the same as the formula unit
- Always check that your molecular formula has the **correct relative molecular mass**

Calculating Reacting Masses from Equations

Stoichiometry and Mass Calculations

Stoichiometry uses **balanced equations** to calculate the quantities of reactants and products in chemical reactions.

The **mole ratio** from a balanced equation relates the amounts of substances that react.

Step-by-Step Method

Calculating Reacting Masses

1. Write the **balanced equation**
2. Calculate the **molar masses** of relevant substances
3. Convert the **known mass** to moles
4. Use the **mole ratio** to find moles of unknown substance
5. Convert moles back to **mass**

Worked Examples

Example 1: Mass of Product from Reactant

Calculate the mass of carbon dioxide produced when 12g of carbon reacts completely with excess oxygen.

$$C^{(s)} + O_2^{(g)} \rightarrow CO_2^{(g)}$$

1. Molar masses: C = 12 g/mol, CO_2 = 44 g/mol
2. Moles of C: 12g ÷ 12 g/mol = 1.0 mol
3. Mole ratio: 1 mol C : 1 mol CO_2
4. Moles of CO_2: 1.0 mol
5. Mass of CO_2: 1.0 mol × 44 g/mol =**44g**

Example 2: Mass of Reactant Needed

Calculate the mass of magnesium needed to react completely with 20g of hydrochloric acid.

$$Mg^{(s)} + 2HCl^{(aq)} \rightarrow MgCl_2^{(aq)} + H_2^{(g)}$$

1. Molar masses: Mg = 24 g/mol, HCl = 36.5 g/mol
2. Moles of HCl: 20g ÷ 36.5 g/mol = 0.55 mol
3. Mole ratio: 1 mol Mg : 2 mol HCl
4. Moles of Mg: 0.55 ÷ 2 = 0.275 mol
5. Mass of Mg: 0.275 mol × 24 g/mol =**6.6g**

Common Mistakes to Avoid

- Always **balance the equation** before doing calculations
- Pay attention to the **mole ratio** - it's not always 1:1
- Use **correct molar masses** for all substances
- Check if the question asks for **excess reactant** or **limiting reactant**
- Remember to include **units** in your final answer

Gas Calculations - Molar Volume

What is Molar Volume?

Molar volume is the volume occupied by one mole of any gas at a specific temperature and pressure.

$V_m = 24\ dm^3\ mol^{-1}$ (at room temperature, 25°C and 1 atm)

$V_m = 22.4\ dm^3\ mol^{-1}$ (at STP, 0°C and 1 atm)

This means that **one mole of any gas** occupies the same volume under the same conditions.

Σ Molar Volume Formula

Key Relationships

```
n = V ÷ Vm
V = n × Vm
```

Where:
- n = number of moles (mol)
- V = volume of gas (dm^3)
- Vm = molar volume ($dm^3\ mol^{-1}$)

Worked Examples

Example 1: Converting Volume to Moles

Calculate the number of moles in 12 dm^3 of oxygen gas at room temperature.

1. Identify the formula: n = V ÷ Vm
2. Substitute values: n = 12 dm^3 ÷ 24 $dm^3\ mol^{-1}$
3. Calculate: n = **0.5 mol**

Example 2: Converting Moles to Volume

Calculate the volume occupied by 2.5 moles of carbon dioxide at room temperature.

1. Identify the formula: V = n × Vm
2. Substitute values: V = 2.5 mol × 24 $dm^3\ mol^{-1}$
3. Calculate: V = **60 dm^3**

Example 3: Using Chemical Equations

Calculate the volume of hydrogen gas produced when 0.8 g of magnesium reacts with excess hydrochloric acid.

1. Equation: $Mg + 2HCl \rightarrow MgCl_2 + H_2$
2. Moles of Mg: 0.8 g ÷ 24 g/mol = 0.033 mol
3. Mole ratio: 1 mol Mg : 1 mol H_2
4. Moles of H_2: 0.033 mol
5. Volume of H_2: 0.033 mol × 24 $dm^3\ mol^{-1}$ = **0.79 dm^3**

Important Points

- Always check the **temperature and pressure conditions** to use the correct molar volume
- Remember that **1 dm^3 = 1000 cm^3 = 1 liter**
- The molar volume is the **same for all gases** under the same conditions
- When using gas volumes in calculations, ensure the **equation is balanced**

Gas Calculations - Ideal Gas Equation

Σ The Ideal Gas Equation

$pV = nRT$

This equation relates the pressure, volume, temperature, and amount of gas.

Variable	Symbol	Units	Description
Pressure	p	Pascal (Pa) or atm	Force per unit area
Volume	V	m^3 or dm^3	Space occupied by gas

Amount	n	moles (mol)	Quantity of gas
Gas constant	R	8.31 J mol^{-1} K^{-1}	Universal constant
Temperature	T	Kelvin (K)	Absolute temperature

Worked Examples

Example 1: Calculating Volume

Calculate the volume of 2.5 moles of gas at 25°C and 1 atm pressure.

1. Convert temperature: T = 25°C + 273 = 298 K
2. Rearrange equation: V = nRT/p
3. Substitute values: V = 2.5 mol × 8.31 J mol^{-1} K^{-1} × 298 K ÷ 101325 Pa
4. Calculate: V = **0.061 m^3** or **61 dm^3**

Example 2: Calculating Pressure

Calculate the pressure of 0.75 moles of gas in a 10 dm^3 container at 300 K.

1. Convert volume: V = 10 dm^3 = 0.010 m^3
2. Rearrange equation: p = nRT/V
3. Substitute values: p = 0.75 mol × 8.31 J mol^{-1} K^{-1} × 300 K ÷ 0.010 m^3
4. Calculate: p = **186975 Pa** or **1.85 atm**

Combined Gas Law

When the amount of gas is constant, we can derive the combined gas law:

$$p_1V_1/T_1 = p_2V_2/T_2$$

> This relates the initial and final states of a gas when conditions change.

> ### Example: Gas Expansion
>
> A gas occupies 20 dm^3 at 1 atm and 300 K. What volume will it occupy at 2 atm and 400 K?
>
> 1. Rearrange equation: $V_2 = p_1V_1T_2/p_2T_1$
> 2. Substitute values: $V_2 = 1\ atm \times 20\ dm^3 \times 400\ K \div (2\ atm \times 300\ K)$
> 3. Calculate: $V_2 =$ **13.3 dm^3**

Important Points

- Always convert temperature to **Kelvin** (K = °C + 273)
- Ensure all units are **consistent** - use SI units (Pa, m^3, K)
- The ideal gas equation works best for **low pressure** and **high temperature** conditions
- For real gases at high pressure or low temperature, corrections may be needed

Percentage Yield Calculations

% What is Percentage Yield?

Percentage yield compares the actual amount of product obtained in a reaction to the theoretical maximum amount that could be produced.

> ### Percentage Yield = (Actual Yield ÷ Theoretical Yield) × 100%
>
> Expressed as a percentage, it measures the efficiency of a reaction.

Theoretical vs. Actual Yield

Theoretical Yield

- **Maximum possible** amount of product
- Calculated from **stoichiometry**
- Assumes **100% conversion**
- No side reactions or losses

Actual Yield

- **Measured amount** of product obtained
- Determined **experimentally**
- Usually **less than** theoretical yield
- Accounts for real-world limitations

Worked Example

Example: Reaction of Sodium with Water

$2Na(s) + 2H_2O(l) \rightarrow 2NaOH(aq) + H_2(g)$

If 4.6g of sodium reacts with excess water and 6.0g of sodium hydroxide is produced, calculate the percentage yield.

1. Calculate moles of Na: 4.6g ÷ 23g/mol = 0.20 mol
2. Mole ratio: 2 mol Na : 2 mol NaOH (1:1)
3. Theoretical moles of NaOH: 0.20 mol
4. Theoretical mass of NaOH: 0.20 mol × 40g/mol = 8.0g
5. Percentage yield: (6.0g ÷ 8.0g) × 100% = **75%**

Why Actual Yields Are Often Lower

- **Incomplete reactions** - not all reactants may convert to products
- **Side reactions** - competing reactions produce other products
- **Product loss** during transfer, purification, or measurement
- **Impurities** in reactants or products
- **Equilibrium limitations** - reversible reactions may not go to completion

Atom Economy Calculations

What is Atom Economy?

Atom economy measures how efficiently atoms in reactants are converted into desired products in a chemical reaction.

> **Atom Economy = (Molar Mass of Desired Product ÷ Sum of Molar Masses of All Products) × 100%**
>
> Unlike percentage yield, atom economy is a theoretical value that doesn't depend on experimental conditions.

Atom Economy vs. Percentage Yield

Atom Economy

- **Theoretical** calculation
- Based on **balanced equation**
- Measures **efficiency** of reaction
- Independent of experimental conditions

Percentage Yield

- **Experimental** measurement
- Based on **actual results**
- Measures **success** of reaction
- Depends on experimental conditions

Worked Example

Example: Production of Ethanol

$C_2H_5Br + NaOH \rightarrow C_2H_5OH + NaBr$

Calculate the atom economy for this reaction if ethanol is the desired product.

1. Molar masses: C_2H_5OH = 46 g/mol, NaBr = 103 g/mol
2. Sum of molar masses of all products: 46 + 103 = 149 g/mol
3. Atom economy = (46 ÷ 149) × 100%

4. Atom economy = **30.9%**

Example: Alternative Production Method

$C_2H_4 + H_2O \rightarrow C_2H_5OH$

Calculate the atom economy for this alternative method.

1. Molar mass of product: C_2H_5OH = 46 g/mol
2. Sum of molar masses of all products: 46 g/mol (only one product)
3. Atom economy = (46 ÷ 46) × 100%
4. Atom economy = **100%**

Importance in Green Chemistry

- High atom economy means **less waste** and more efficient use of resources
- Reduces the need for **waste disposal** and minimizes environmental impact
- Important consideration in **industrial processes** for sustainability
- Reactions with high atom economy are often more **economically viable**
- Key principle of **green chemistry** - designing reactions that minimize waste

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Core Practical 1 - Measurement of the Molar Volume of a Gas

Purpose and Reaction

To determine the **molar volume** of a gas by collecting and measuring the volume of hydrogen gas produced from the reaction between magnesium and hydrochloric acid.

$$Mg^{(s)} + 2HCl^{(aq)} \rightarrow MgCl_2^{(aq)} + H_2^{(g)}$$

Apparatus Required

Equipment

- Conical flask with delivery tube
- Measuring cylinder (inverted) or gas syringe
- Water trough
- Balance (accurate to 0.01g)
- Thermometer
- Ruler or measuring tape

Experimental Procedure

Method

1. Weigh a known mass of magnesium ribbon (e.g., 0.12g)
2. Set up apparatus with inverted measuring cylinder filled with water
3. Add excess dilute HCl to magnesium in conical flask
4. Collect hydrogen gas over water until reaction completes
5. Record volume of gas collected and temperature

Calculations

1. Calculate moles of Mg: n = mass ÷ molar mass
2. From equation, 1 mol Mg produces 1 mol H_2
3. Calculate molar volume: Vm = volume of H_2 ÷ moles of H_2
4. Adjust for water vapor pressure if needed
5. Convert to standard conditions if required

Safety Precautions

- Wear **safety goggles** and lab coat
- Handle **hydrochloric acid** with care
- Ensure good **ventilation** as hydrogen is flammable
- Check for **leaks** in the apparatus before starting

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Displacement Reactions and Equations

What are Displacement Reactions?

Reactions where an element in a compound is **replaced** by another element.

Single Displacement

- One element replaces another
- More reactive element displaces less reactive
- General form: A + BC ⟶ AC + B

Double Displacement

- Parts of two compounds exchange
- Often forms precipitate or gas
- General form: AB + CD ⟶ AD + CB

Single Displacement Examples

Metal Displacement

Zinc displaces copper from copper(II) sulfate solution:

$$Zn^{(s)} + CuSO_4{}^{(aq)} \rightarrow ZnSO_4{}^{(aq)} + Cu^{(s)}$$

Observations

- Blue solution turns colorless
- Reddish-brown copper metal deposits
- Zinc metal dissolves

Halogen Displacement

Chlorine displaces bromine from potassium bromide:

$$Cl_2{}^{(g)} + 2KBr^{(aq)} \rightarrow 2KCl^{(aq)} + Br_2{}^{(l)}$$

Observations

- Colorless solution turns orange-brown
- Bromine liquid forms at bottom

Double Displacement Examples

Precipitation Reaction

Silver nitrate reacts with sodium chloride:

$$AgNO_3{}^{(aq)} + NaCl^{(aq)} \rightarrow AgCl^{(s)} + NaNO_3{}^{(aq)}$$

Observations

- White precipitate of silver chloride forms
- Solution remains clear

Acid-Base Reaction

Hydrochloric acid reacts with sodium hydroxide:

$$HCl^{(aq)} + NaOH^{(aq)} \rightarrow NaCl^{(aq)} + H_2O^{(l)}$$

Observations

- Neutralization occurs
- Temperature increases (exothermic)
- Solution remains clear

Acid Reactions and Equations

Acid Properties

Acids are substances that **donate protons (H^+)** in aqueous solution. They react with various substances in predictable patterns.

Types of Acid Reactions

Acid + Metal

Acids react with reactive metals to produce hydrogen gas and a salt.

$$2HCl_{(aq)} + Zn_{(s)} \rightarrow ZnCl_{2(aq)} + H_{2(g)}$$

Observations

- Bubbles of gas form
- Metal dissolves
- Solution may heat up

Acid + Metal Oxide

Acids react with metal oxides to produce salt and water.

$$2HCl_{(aq)} + CuO_{(s)} \rightarrow CuCl_{2(aq)} + H_2O_{(l)}$$

Observations

- Solid dissolves
- Solution may change color
- Temperature may increase

Acid + Metal Hydroxide

Acids react with metal hydroxides (bases) in neutralization reactions.

$$H_2SO_{4(aq)} + 2NaOH_{(aq)} \rightarrow Na_2SO_{4(aq)} + 2H_2O_{(l)}$$

Observations

Acid + Carbonate

Acids react with carbonates to produce salt, water, and carbon dioxide.

$$2HCl_{(aq)} + CaCO_{3(s)} \rightarrow CaCl_{2(aq)} + H_2O_{(l)} + CO_{2(g)}$$

Observations

- Bubbles of gas form

- Solution may become neutral (pH 7)
- Temperature increases (exothermic)
- No visible change if both solutions are colorless

- Solid dissolves
- Gas turns limewater milky

Key Points for Writing Acid Equations

Writing Balanced Equations

- Identify the **type of reaction** based on reactants
- Predict the **products** using the reaction patterns
- Include **state symbols** (s, l, g, aq)
- **Balance** the equation to conserve atoms
- Remember that acids always produce **H^+ ions** in solution

Precipitation Reactions and Equations

What are Precipitation Reactions?

Reactions where two aqueous solutions combine to form an **insoluble solid** (precipitate).

These are a type of **double displacement** reaction where ions exchange partners.

Solubility Rules

Generally Soluble

- All **Group 1** metal compounds (Na^+, K^+, etc.)
- All **ammonium** compounds (NH_4^+)

- All **nitrate** compounds (NO_3^-)
- Most **chloride** compounds (except Ag^+, Pb^{2+})

Generally Insoluble

- Most **carbonate** compounds (except Group 1, NH_4^+)
- Most **hydroxide** compounds (except Group 1, NH_4^+)
- Most **sulfide** compounds (except Group 1, NH_4^+)
- Most **phosphate** compounds (except Group 1, NH_4^+)

Examples of Precipitation Reactions

Silver Nitrate + Sodium Chloride

When solutions of silver nitrate and sodium chloride are mixed:

$$AgNO_3{}^{(aq)} + NaCl^{(aq)} \rightarrow AgCl^{(s)} + NaNO_3{}^{(aq)}$$

Observations

- **White precipitate** of silver chloride forms
- Solution remains clear (sodium nitrate is soluble)

Lead(II) Nitrate + Potassium Iodide

When solutions of lead(II) nitrate and potassium iodide are mixed:

$$Pb(NO_3)_2{}^{(aq)} + 2KI^{(aq)} \rightarrow PbI_2{}^{(s)} + 2KNO_3{}^{(aq)}$$

Observations

- **Yellow precipitate** of lead(II) iodide forms
- Solution remains clear (potassium nitrate is soluble)

Writing Precipitation Equations

Key Steps

> - Identify the **ions** present in each reactant
> - Predict the **products** by exchanging ions
> - Use **solubility rules** to determine which product is insoluble
> - Write the **balanced equation** with correct state symbols
> - Remember that **spectator ions** remain in solution