LEARNERS' ALLEY
Designed by Khow Willard

4 Chemical Formulae, Equations, the Mole and Gases

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Atoms are far too small to count one by one, yet chemists need to know exactly how much of each substance reacts. This chapter writes reactions as balanced equations, counts particles in moles, and uses moles to work out masses, concentrations and gas volumes.

Learning objectives

By the end of this chapter, you can:

Foundation O LEVEL

- write balanced equations with state symbols, and ionic equations
- calculate A_r, M_r, moles, masses and numbers of particles
- find empirical and molecular formulae
- use mole ratios for reacting masses, limiting reagents, percentage yield and purity
- use concentrations and the molar gas volume

Core A LEVEL

- calculate A_r from isotopic abundances
- find a formula from combustion data
- use $pV = nRT$, including M_r and density of a gas
- use Dalton's law of partial pressures
- state the ideal gas assumptions and explain when real gases deviate

Prerequisites

Chapter 1 (particles, diffusion, states of matter), Chapter 2 (isotopes and the mole as a counting unit) and Chapter 3 (ions, ionic formulae and intermolecular forces). Fill in the blanks as the lesson goes.

4.1 Chemical equations

A chemical equation shows the reactants on the left and the products on the right. Atoms are not created or destroyed in a reaction, so a **balanced equation** has the same number of each kind of atom on both sides. Balance an equation by changing the numbers in front of the formulae, never the formulae themselves.

WORKED EXAMPLE Balance the equation for burning methane: $CH_4 + O_2 \rightarrow CO_2 + H_2O$.

1. C: 1 on each side already.	*Start with an element that appears in one formula on each side.*
2. H: 4 on the left, so $2H_2O$ on the right.	*$CH_4 + O_2 \rightarrow CO_2 + 2H_2O$*
3. O: 2 + 2 = 4 on the right, so $2O_2$: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$	*Balance the free element last.*

State symbols show the state of each substance: (s) solid, (l) liquid, (g) gas and (aq) aqueous, dissolved in water.

4.1.1 Ionic equations

An ionic compound dissolved in water is present as separate ions. An **ionic equation** shows only the particles that change. Ions that are in the same state on both sides take no part, and are called **spectator ions**.

1. Write the balanced equation with state symbols.
2. Split every aqueous ionic compound into its ions. Solids, liquids, gases and covalent molecules stay whole.
3. Cross out the ions that appear unchanged on both sides.

WORKED EXAMPLE Write the ionic equation for $AgNO_3(aq) + NaCl(aq) \rightarrow AgCl(s) + NaNO_3(aq)$.

1. $Ag^+(aq) + NO_3^-(aq) + Na^+(aq) + Cl^-(aq) \rightarrow AgCl(s) + Na^+(aq) + NO_3^-(aq)$	*AgCl is a solid, so it stays whole.*
2. Na^+ and NO_3^- are spectators.	*Unchanged on both sides.*
$Ag^+(aq) + Cl^-(aq) \rightarrow AgCl(s)$	*Charges also balance: 0 on each side.*

A metal placed in a solution of another metal's ions works the same way: $Mg(s) + CuSO_4(aq) \rightarrow MgSO_4(aq) + Cu(s)$ becomes $Mg(s) + Cu^{2+}(aq) \rightarrow Mg^{2+}(aq) + Cu(s)$. An ionic equation must balance in charge as well as atoms.

Check your understanding

1. Balance: $Al + O_2 \rightarrow Al_2O_3$.
2. Write the ionic equation for $BaCl_2(aq) + Na_2SO_4(aq) \rightarrow BaSO_4(s) + 2NaCl(aq)$.

4.2 Relative masses

Atoms are compared with the carbon-12 atom, which is given a mass of exactly 12. Relative masses have no units.

DEFINITION The **relative atomic mass**, A_r, of an element is the _____ mass of one atom of the element compared with 1/12 of the mass of one atom of carbon-12. The **relative molecular mass**, M_r, is the same comparison for a molecule. For an ionic compound it is called the relative formula mass, also written M_r.

M_r is the sum of the A_r of all the atoms in the formula. Values of A_r are given in the Periodic Table: for CO_2, M_r = 12.0 + 2(16.0) = _____. For $Ca(NO_3)_2$, M_r = 40.1 + 2(14.0 + 3 × 16.0) = 164.1.

The **percentage by mass** of an element in a compound is the total A_r of that element in the formula divided by M_r, × 100%. In CO_2, carbon is 12.0 ÷ 44.0 × 100% = 27.3% by mass.

4.2.1 A_r from isotopes CORE · A LEVEL

A_r is rarely a whole number because it averages the isotopes, weighted by how common each is (Figure 4.1).

$$A_r = \frac{\Sigma\ (\text{percentage abundance} \times \text{isotopic mass})}{100}$$

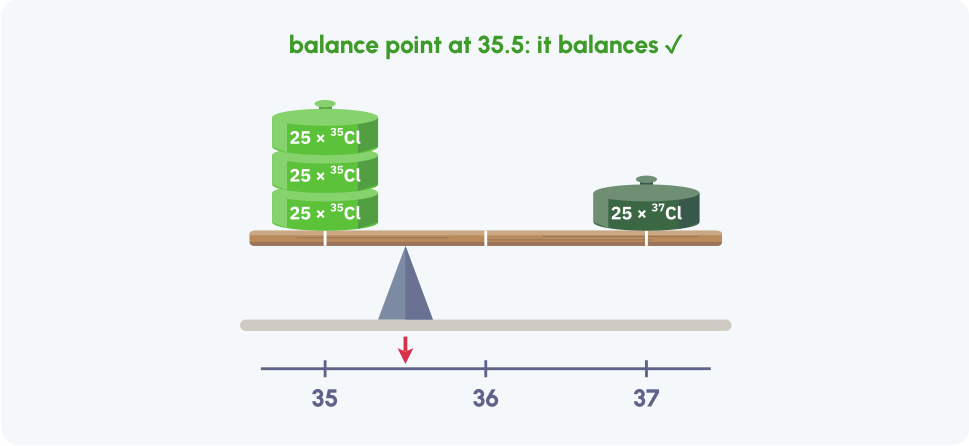


Figure 4.1 A weighted average: balanced at 36 the plank tips, as three in four chlorine atoms are chlorine-35; it balances at 35.5.

WORKED EXAMPLE Chlorine is 75.77% ^{35}Cl and 24.23% ^{37}Cl. Calculate A_r(Cl).

A_r = (75.77 × 35 + 24.23 × 37) ÷ 100 = _____ *Weight each isotope by its abundance.*

Check your understanding

1. Calculate M_r of $(NH_4)_2SO_4$. (A_r: H 1.0, N 14.0, O 16.0, S 32.1)
2. Copper is 69% ^{63}Cu and 31% ^{65}Cu. Calculate A_r(Cu).

4.3 The mole

DEFINITION A **mole** is the amount of substance containing 6.02×10^{23} particles. This number is the **Avogadro constant**, L. The **molar mass**, M, is the mass of one mole of a substance in g mol^{-1}. It is numerically equal to A_r or M_r.

WHY THE MOLE MATTERS Atoms are far too small to count or weigh one at a time, but a balance measures grams. The mole is the bridge between the two. A proton and a neutron each have a mass of about 1 on the relative scale. Chemists asked how many of these units it takes to make _____, a mass we can actually weigh. The answer is 6.02×10^{23}: that many protons weigh about 1 g (the exact definition uses carbon-12, so 6.02×10^{23} carbon-12 atoms weigh exactly 12 g).

We already know how heavy every atom is in these units: its A_r. So a mole of any substance weighs its A_r or M_r in grams. One mole of carbon-12 atoms has a mass of exactly 12 g, one mole of oxygen atoms 16.0 g, and one mole of water molecules (M_r 18.0) 18.0 g. Each of these samples contains the same number of particles, 6.02×10^{23}. Weighing out 18.0 g of water is therefore a way of counting out 6.02×10^{23} molecules. Always say which particle you are counting: 1 mol of O_2 molecules contains 2 mol of O atoms.

$$\text{amount (mol) } n = \frac{\text{mass (g)}}{\text{molar mass (g mol}^{-1})} \qquad \text{number of particles } N = n \times L$$

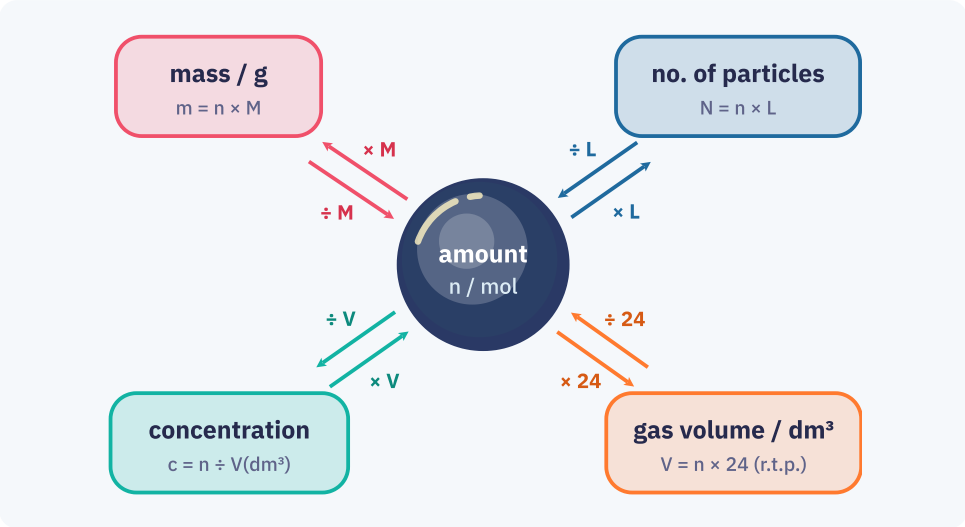


Figure 4.2 Every calculation goes through the amount in moles.

WORKED EXAMPLE How many molecules, and how many atoms, are in 4.40 g of carbon dioxide?

1. $n = 4.40 \div 44.0 = 0.100$ mol CO_2 — *Mass to moles.*
2. Molecules $= 0.100 \times 6.02 \times 10^{23} = 6.02 \times 10^{22}$ — *Moles to particles.*
3. Atoms $= 3 \times 6.02 \times 10^{22} =$ _____ — *Each CO_2 has 3 atoms.*

EXAM TIP Keep 4 significant figures in working and give the answer to 3 significant figures unless told otherwise. A value read from the Periodic Table, such as $A_r(O) = 16.0$, has 3.

Check your understanding

1. What is the mass of 0.250 mol of sodium hydroxide, NaOH? (A_r: Na 23.0, O 16.0, H 1.0)

2. How many chloride ions are in 0.10 mol of $CaCl_2$?

4.4 Empirical and molecular formulae

DEFINITION The **empirical formula** shows the _____ of the atoms in a compound. The **molecular formula** shows the actual number of each atom in one molecule.

Glucose has the molecular formula $C_6H_{12}O_6$ and the empirical formula CH_2O. The molecular formula is a whole-number multiple of the empirical formula: multiple = $M_r \div$ empirical formula mass.

WORKED EXAMPLE Compound X (M_r 114) is 63.2% C, 12.2% H and 24.6% N by mass. Find its molecular formula.

	C	H	N
mass in 100 g / g	63.2	12.2	24.6
amount / mol (÷ A_r)	5.267	12.20	1.757
ratio (÷ 1.757)			

Empirical C_3H_7N (mass 57.0). 114 ÷ 57.0 = 2, so $C_6H_{14}N_2$.

Take 100 g so each percentage becomes a mass.

4.4.1 Formulae from combustion CORE · A LEVEL

When a compound of carbon, hydrogen and oxygen burns completely in oxygen, all its carbon ends up in CO_2 and all its hydrogen in H_2O (Figure 4.3). The oxygen cannot be found this way, because some of the oxygen in the products came from the O_2. Find it by difference.

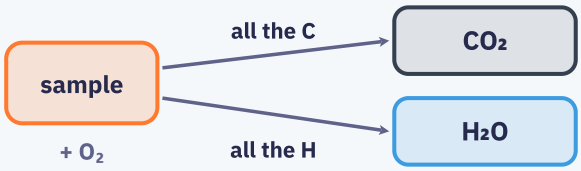


Figure 4.3 Where the carbon and hydrogen go on combustion.

WORKED EXAMPLE 2.36 g of a sugar (C, H and O only, M_r 180) burns completely to give 3.46 g of CO_2 and 1.42 g of H_2O. Find its molecular formula.

1. C: 12/44 × 3.46 = 0.9436 g. H: 2/18 × 1.42 = 0.1578 g. — *12 g of C in every 44 g of CO_2, 2 g of H in every 18 g of H_2O.*
2. O: 2.36 − 0.9436 − 0.1578 = 1.259 g — *By difference.*
3. Moles: C 0.07863, H 0.1578, O 0.07869, ratio 1 : 2 : 1 — *Empirical formula CH_2O (mass 30).*
4. 180 ÷ 30 = 6, so $C_6H_{12}O_6$. — *Multiply up.*

Check your understanding

1. A compound is 85.7% C and 14.3% H by mass, and M_r is 56. Find its molecular formula.

4.5 Reacting masses

The numbers in a balanced equation give the _____ of the substances. $2H_2 + O_2 \rightarrow 2H_2O$ means 2 mol of H_2 react with 1 mol of O_2 to give 2 mol of H_2O. To find a reacting mass: mass to moles, moles across by the ratio, then moles back to mass.

WORKED EXAMPLE What mass of magnesium oxide forms when 6.0 g of magnesium burns completely? $2Mg + O_2 \rightarrow 2MgO$ (A_r: Mg 24.0, O 16.0)

1. $n_{Mg} = 6.0 \div 24.0 = 0.25$ mol	*Mass to moles.*
2. $n_{MgO} = 0.25$ mol	*Ratio 2 : 2.*
3. mass = 0.25×40.0 = _____	*Moles to mass.*

4.5.1 Limiting reagent and yield

The **limiting reagent** is the reactant that is used up first. It fixes the greatest amount of product that can form, the **theoretical yield**. The other reactant is in **excess** (Figure 4.4).

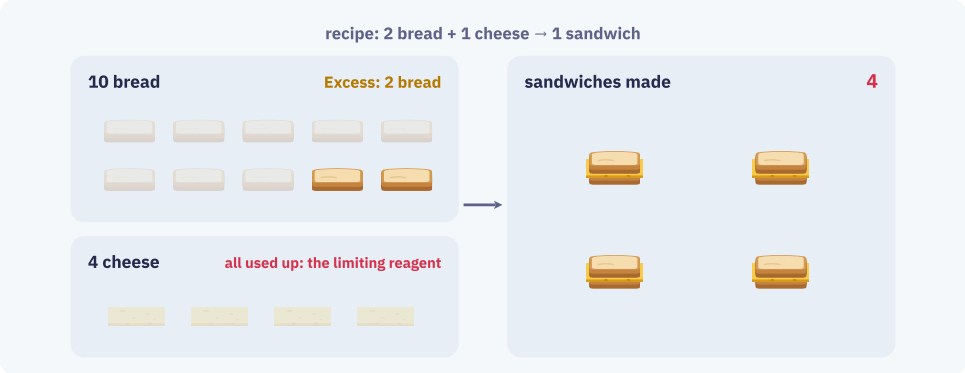


Figure 4.4 The cheese limits the number of sandwiches. The bread is in excess.

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% \qquad \text{percentage purity} = \frac{\text{mass of pure substance}}{\text{mass of impure sample}} \times 100\%$$

WORKED EXAMPLE 2.4 g of magnesium is heated with 0.80 g of oxygen. $2Mg + O_2 \rightarrow 2MgO$. 1.6 g of MgO is collected. Find the limiting reagent and the percentage yield.

1. $n_{Mg} = 2.4 \div 24.0 = 0.10$ mol. $n_{O_2} = 0.80 \div 32.0 = 0.025$ mol.	*Convert both to moles.*
2. 0.10 mol Mg needs 0.050 mol O_2, but only 0.025 mol is present, so O_2 is limiting.	*Compare with the ratio 2 : 1.*
3. $n_{MgO} = 2 \times 0.025 = 0.050$ mol, theoretical yield $= 0.050 \times 40.0 = 2.0$ g	*Work from the limiting reagent.*
4. % yield = $1.6 \div 2.0 \times 100\%$ = _____	*Actual ÷ theoretical.*

Check your understanding

1. Calcium carbonate decomposes on heating: $CaCO_3 \rightarrow CaO + CO_2$. What mass of CaO forms from 25.0 g of $CaCO_3$? (A_r: Ca 40.1, C 12.0, O 16.0)
2. A 5.00 g sample of impure $CaCO_3$ gives 1.76 g of CO_2. What is its percentage purity?

4.6 Solutions

DEFINITION The **concentration** of a solution is the amount of solute in 1 dm^3 of solution, in mol dm^{-3}, or the mass of solute in 1 dm^3, in g dm^{-3}.

$$\text{concentration (mol dm}^{-3}) = \frac{\text{amount (mol)}}{\text{volume (dm}^3)} \qquad 1\ dm^3 = 1000\ cm^3$$

To make a solution of known concentration, weigh the solute, dissolve it in a little water, transfer it to a volumetric flask and add water up to the mark (Figure 4.5). Adding water to a solution **dilutes** it: the amount of solute stays the same, so $c_1V_1 = c_2V_2$.



Figure 4.5 Making a solution of known concentration.

WORKED EXAMPLE 4.00 g of sodium hydroxide (M_r 40.0) is dissolved to make 250 cm^3 of solution. Find its concentration. What volume of water must be added to 50.0 cm^3 of it to make a 0.100 mol dm^{-3} solution?

1. n = 4.00 ÷ 40.0 = 0.100 mol, c = 0.100 ÷ 0.250 = _____ — *Convert 250 cm^3 to 0.250 dm^3.*
2. 0.400 × 50.0 = 0.100 × V_2, so V_2 = 200 cm^3 — *$c_1V_1 = c_2V_2$*
3. Water to add = 200 − 50.0 = _____ — *V_2 is the final total volume.*

Check your understanding

1. How many moles of solute are in 25.0 cm^3 of 0.200 mol dm^{-3} solution?

2. Express 0.500 mol dm^{-3} sodium chloride (M_r 58.5) in g dm^{-3}.

4.7 Gas volumes

DEFINITION **Avogadro's law**: at the same temperature and pressure, equal volumes of all gases contain the same number of particles. So one mole of any gas occupies the same volume, the **molar gas volume**: _____ at room temperature and pressure (r.t.p.).

- volume of gas (dm^3) = amount (mol) × 24 at r.t.p. At standard conditions (s.t.p., 0 °C and 1 bar) one mole occupies 22.7 dm^3. Use the value for the conditions the question gives.
- For gases at the same temperature and pressure, the _____ equals the mole ratio. Only gases count: a liquid such as water at r.t.p. takes up almost no volume.

WORKED EXAMPLE What volume of hydrogen at r.t.p. forms when 0.230 g of sodium reacts with excess water? $2Na + 2H_2O \rightarrow 2NaOH + H_2$

1. $n_{Na} = 0.230 \div 23.0 = 0.0100$ mol — *Water is in excess, so Na is limiting.*
2. $n_{H_2} = 0.00500$ mol — *Ratio 2 : 1.*
3. $V = 0.00500 \times 24 = 0.120$ dm^3 = _____ — *Molar gas volume at r.t.p.*

4.7.1 Burning gaseous hydrocarbons

A hydrocarbon C_xH_y burns completely to carbon dioxide and water: $C_xH_y + (x + y/4)O_2 \rightarrow xCO_2 + (y/2)H_2O$. After cooling to room temperature the water is liquid, so the gas volume shrinks. Aqueous sodium hydroxide absorbs carbon dioxide, so passing the gas through it removes the CO_2 and shows its volume (Figure 4.6).

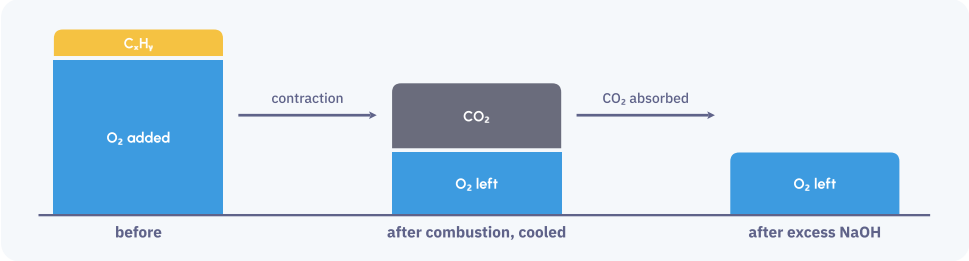


Figure 4.6 Following the gas volumes when a hydrocarbon burns. Bar lengths are drawn for illustration.

WORKED EXAMPLE 10 cm^3 of a gaseous hydrocarbon is burnt in 110 cm^3 of oxygen (excess). After cooling to r.t.p. the volume is 85 cm^3, falling to 35 cm^3 after passing through aqueous sodium hydroxide. Find the formula of the hydrocarbon.

1. $V(CO_2) = 85 - 35 = 50$ cm^3 $= 10x$, so $x = 5$ — *NaOH removes the CO_2.*
2. O_2 used $= 110 - 35 = 75$ cm^3 $= 10(x + y/4)$ — *The 35 cm^3 left is unused O_2.*
3. $7.5 = 5 + y/4$, so $y = 10$: _____ — *Volume ratio = mole ratio.*

Check your understanding

1. What volume does 8.0 g of oxygen gas, O_2, occupy at r.t.p.?

2. What volume of oxygen is needed to burn 20 cm^3 of methane completely? $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

4.8 The ideal gas equation

CORE · A LEVEL

A gas exerts **pressure** because its particles collide with the walls of the container: pressure is the force of these collisions per unit area (Figure 4.7). For a fixed amount of gas, pressure rises when the volume falls (the particles travel a shorter distance between collisions with the walls, so they hit the walls more often) and when the temperature rises (faster particles hit harder and more often).

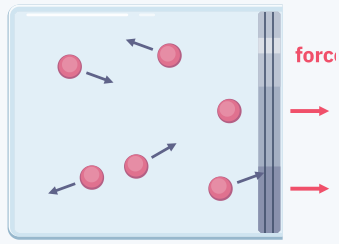


Figure 4.7 Each collision pushes on the wall.

The **ideal gas equation** is $pV = nRT$, with every quantity in SI units: p in Pa, V in m^3, n in mol, T in K, and the gas constant $R = 8.31\ J\ K^{-1}\ mol^{-1}$.

WHAT THE EQUATION SAYS Pressure, volume, amount and temperature are the four things you can measure about a gas. For every ideal gas they are tied together: pV ÷ nT always comes out to the _____, R. So the four cannot change independently. If you know any _____, the equation gives the fourth.

quantity	SI unit	conversions
pressure	Pa	1 atm = 101 325 Pa, 1 bar = 10^5 Pa, 1 kPa = 10^3 Pa
volume	m^3	1 dm^3 = 10^{-3} m^3, 1 cm^3 = _____ m^3
temperature	K	T / K = T / °C + 273

- Substituting n = m ÷ M_r gives **M_r = mRT ÷ pV**, so a gas's M_r can be found from its mass, volume, temperature and pressure.
- For a fixed amount of gas, $p_1V_1/T_1 = p_2V_2/T_2$. At constant temperature pV is constant (Boyle's law). At constant pressure V ∝ T (Charles's law).

WORKED EXAMPLE 0.10 g of a gas occupies 83.1 cm^3 at 1.0×10^5 Pa and 27 °C. Find its M_r.

1. $V = 83.1 \times 10^{-6}\ m^3$, T = 300 K — *Convert to SI units first.*

2. $M_r = (0.10 \times 8.31 \times 300) \div (1.0 \times 10^5 \times 83.1 \times 10^{-6})$ — *$M_r = mRT \div pV$*
= _____

4.8.1 Dalton's law of partial pressures

In a mixture of gases that do not react, each gas behaves as if it were alone (Figure 4.8).

The **partial pressure** of a gas in a mixture is the pressure it would exert if it alone occupied the container. **Dalton's law**: the total pressure is the _____ of the partial pressures, $p_{total} = p_A + p_B + \ldots$

A gas's share of the pressure equals its share of the particles: $p_A = x_A \times p_{total}$, where the **mole fraction** $x_A = n_A \div n_{total}$.

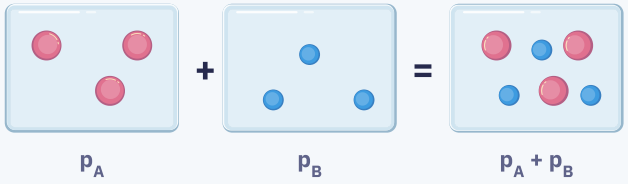


Figure 4.8 Dalton's law.

WORKED EXAMPLE A 1 dm^3 flask of helium at 2 kPa is joined to a 2 dm^3 flask of neon at 1 kPa at constant temperature (Figure 4.9). Find the final total pressure.

1. He spreads into 3 dm^3: $p_{He} = 2 \times 1/3 = 0.667$ kPa — *Boyle's law for each gas alone.*
2. Ne spreads into 3 dm^3: $p_{Ne} = 1 \times 2/3 = 0.667$ kPa — *pV is constant.*
3. $p_{total} = 0.667 + 0.667 =$ _____ — *Dalton's law.*

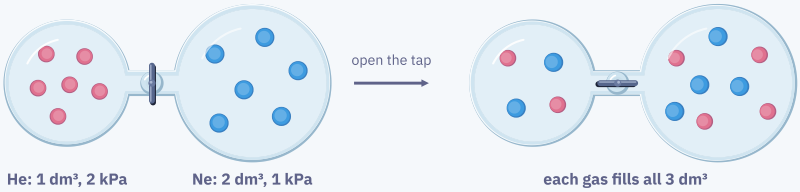


Figure 4.9 Two flasks joined by a tap, before and after it opens.

4.8.2 Ideal and real gases

An **ideal gas** obeys pV = nRT exactly. The kinetic theory explains its behaviour with these assumptions (Figure 4.10):

1. The particles have _____ compared with the container.
2. There are _____ between the particles.
3. The particles move randomly, and their collisions lose no kinetic energy.

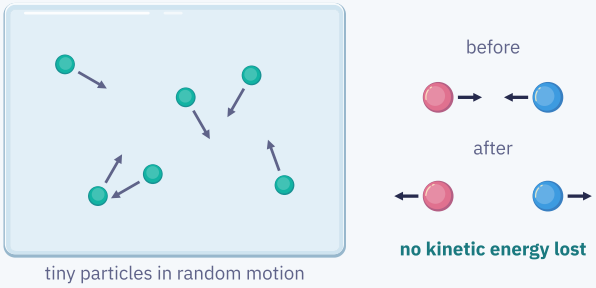


Figure 4.10 The ideal gas model.

Real gases come closest to ideal at _____ and _____, where the particles are fast and far apart. They deviate most at low temperature and high pressure, for two reasons (Figure 4.11):

- **Intermolecular forces**: a particle about to hit the wall is pulled back by its neighbours, so it hits more gently and pV is less than ideal. Stronger intermolecular forces give a larger deviation.
- **Particle volume**: at high pressure the particles take up a real share of the container, so the gas occupies more volume than an ideal gas would and pV is more than ideal.

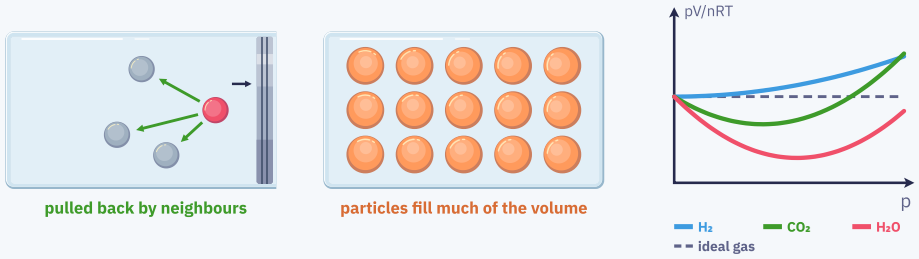


Figure 4.11 Why real gases deviate, and pV/nRT against p for three gases (shapes for illustration). The more strongly the molecules attract, the larger the dip.

WORKED EXAMPLE Put CH_4, HCl and HF in order, most ideal first, under the same conditions.

1. CH_4 has only instantaneous dipole–induced dipole forces, HCl also has permanent dipole–permanent dipole forces, and HF has hydrogen bonds. *Chapter 3 intermolecular forces.*

2. Stronger forces mean more deviation: CH_4 > HCl > HF. *The weakest forces behave most ideally.*

Check your understanding

1. What volume, in dm^3, does 1.00 mol of an ideal gas occupy at 0 °C and 1.00×10^5 Pa?

2. A mixture contains 0.5 mol He and 1.5 mol Ar at a total pressure of 200 kPa. Find the partial pressure of He.

3. Why does helium behave more ideally than ammonia?

Answers to Check your understanding

4.1

1. $4Al + 3O_2 \rightarrow 2Al_2O_3$
2. $Ba^{2+}(aq) + SO_4^{2-}(aq) \rightarrow BaSO_4(s)$. Na^+ and Cl^- are spectators.

4.2

1. $2(14.0 + 4 \times 1.0) + 32.1 + 4 \times 16.0 = 132.1$
2. $(69 \times 63 + 31 \times 65) \div 100 = 63.6$

4.3

1. $M_r = 40.0$, mass = $0.250 \times 40.0 = 10.0$ g
2. $0.10 \times 2 = 0.20$ mol of Cl^-, which is $0.20 \times 6.02 \times 10^{23} = 1.2 \times 10^{23}$ ions

4.4

1. C: 85.7 ÷ 12.0 = 7.14, H: 14.3 ÷ 1.0 = 14.3, ratio 1 : 2, empirical CH_2 (14). 56 ÷ 14 = 4, so C_4H_8.

4.5

1. $n_{CaCO_3} = 25.0 \div 100.1 = 0.2498$ mol, so $n_{CaO} = 0.2498$ mol and mass = $0.2498 \times 56.1 = 14.0$ g

2. $n_{CO_2} = 1.76 \div 44.0 = 0.0400$ mol $= n_{CaCO_3}$. Mass of $CaCO_3 = 0.0400 \times 100.1 = 4.004$ g, purity $= 4.004 \div 5.00 \times 100\% = 80.1\%$

4.6

1. $0.200 \times 0.0250 = 0.00500$ mol
2. $0.500 \times 58.5 = 29.3$ g dm^{-3}

4.7

1. $n = 8.0 \div 32.0 = 0.25$ mol, $V = 0.25 \times 24 = 6.0$ dm^3
2. 40 cm^3: the volume ratio $CH_4 : O_2$ is 1 : 2.

4.8

1. $V = nRT \div p = 1.00 \times 8.31 \times 273 \div 1.00 \times 10^5 = 0.0227$ $m^3 = 22.7$ dm^3
2. $x(He) = 0.5 \div 2.0 = 0.25$, so $p(He) = 0.25 \times 200 = 50$ kPa
3. Helium atoms have only very weak instantaneous dipole–induced dipole forces and a small volume. Ammonia molecules are attracted by hydrogen bonds, so they deviate more.