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Content Guidance

Questions & Answers

Molar gas volume

At 25°C (T = 298 K), atmospheric pressure (p = 101 325 Pa) and using a gas constant, $R = 8.31\,J\,K^{-1}\,mol^{-1}$, the volume of 1 mole ($n$ = 1) of a gas is calculated as:

$$pV = nRT$$

$$V = \frac{nRT}{p} = \frac{1 \times 8.31 \times 298}{101325} = 0.0244\,m^3$$

$$V = 24.4\,dm^3$$

Often $24\,dm^3$ is used as the molar gas volume for 1 mole of any gas at 25°C and atmospheric pressure.

Empirical and molecular formulae

Types of formulae

There are two main types of chemical formulae:

- An **empirical formula** shows the simplest ratio of the atoms of each element.
  This type of formula is used for ionic compounds and macromolecules (giant covalent molecules).
  Examples: NaCl (ionic); MgO (ionic); $CaCl_2$ (ionic); SiO_2 (macromolecular)
- A **molecular formula** shows the actual number of atoms of each element in one molecule of the substance.
  This type of formula is used for all molecular (simple) covalent substances.
  Examples: H_2O; CO_2; O_2; CH_4; NH_3; H_2O_2; I_2; S_8 (all molecular covalent)

Some elements exist as simple molecules. These are the diatomic elements (H_2, N_2, O_2, F_2, Cl_2, Br_2, I_2), sulfur (S_8) and phosphorus (P_4).

The empirical formula states the simplest ratios of all the elements in the compound. For example, ethane has molecular formula C_2H_6 but its empirical formula is CH_3.

The M_r of a substance will be the same as the mass of the atoms in the empirical formula if the empirical formula is the same as the molecular formula, or it will be a simple multiple.

The term molar mass may be used in place of M_r.

The molar mass is the mass of 1 mole and is measured in units of $g\,mol^{-1}$.

Worked example

The empirical formula of a compound is CH. The M_r is determined to be 78.0. What is the molecular formula of the compound?

Answer

empirical formula: CH, empirical formula mass: 13.0, M_r: 78.0

$$\frac{\text{molar mass}}{\text{empirical formula mass}} = \frac{78.0}{13.0} = 6$$

So:

molecular formula = 6 × empirical formula

molecular formula = C_6H_6

Exam tip

The volume of 1 mole of any gas under different conditions may be calculated by changing the temperature or pressure in this calculation.

Knowledge check 9

0.214 mol of chlorine gas were produced during a reaction. Calculate the volume of gas, in dm^3, at 300 K and 100 kPa. The gas constant, $R = 8.31\,J\,K^{-1}\,mol^{-1}$. Give your answer to 3 significant figures.

Exam tip

An empirical formula can be written for molecular covalent substances and this may be the same as the molecular formula or it may be different, for example, the molecular formula of hydrogen peroxide is H_2O_2 but its empirical formula is written as HO (simplest ratio).

Knowledge check 10

What is the empirical formula of $C_6H_4N_2O_4$?

Finding formulae

The empirical formula of a compound may be determined from mass measurements taken during a reaction between two elements or from heating hydrated compounds to constant mass to remove the water of crystallisation. The formula can also be determined from the given percentage composition by mass.

Worked example

0.91 g of titanium combined with oxygen to give 1.52 g of an oxide of titanium. Find the formula of the oxide of titanium.

Practically, this is done by heating a certain mass of titanium in a crucible with a lid, which is raised periodically to let fresh air in. The titanium is heated to constant mass to ensure that all the titanium has combined to form the oxide.

1 Find the mass of the empty crucible: 16.18 g
2 Find the mass of the crucible and some titanium: 17.09 g
3 Mass of titanium = (2) – (1) = 17.09 – 16.18 = 0.91 g
4 Find the mass of the crucible after heating to constant mass: 17.70 g
5 Mass of oxygen combined = (4) – (2) = 17.70 – 17.09 = 0.61 g

Answer

Using this information we can now calculate the formula of the oxide of titanium, as shown in Table 6.

Element	Titanium	Oxygen
Mass (g)	0.91	0.61
A_r	47.9	16.0
Moles	0.91/47.9 = 0.019	0.61/16.0 = 0.038
Ratio	1	2
Formula	TiO_2	

Table 6

As the ratio is one Ti atom to two O atoms, we say that the *empirical formula* is TiO_2, but it could also be Ti_2O_4 or Ti_3O_6, etc., as the ratio in these compounds is the same.

If the moles work out to be not as simple as the ones shown in the example, then to calculate the ratio, divide all the moles by the smallest number of moles. If you end up with, say, 0.5, then multiply all the ratio numbers by 2 to get whole numbers.

Hydrated salts

Many salts (formed from acids) are hydrated when they are solid. A hydrated salt contains **water of crystallisation**.

If hydrated salts are heated to constant mass in an open container (so the water vapour can escape) all of the water of crystallisation is removed, and an **anhydrous salt** remains.

Hydrated salts are written with the water of crystallisation, for example, $CuSO_4.5H_2O$, or $CoCl_2.6H_2O$, or $Na_2CO_3.10H_2O$.

Exam tip

Use the A_r of oxygen as 16.0 as we are dealing with oxygen atoms combined in the formula.

Knowledge check 11

What is the empirical formula of the chloride of mercury when 1.20 g of mercury combines with 0.425 g of chlorine? Determine the empirical formula of the chloride of mercury.

Water of crystallisation refers to water molecules chemically bonded within a crystal structure.

An **anhydrous salt** contains no water of crystallisation.

ⓔ The majority of enthalpy change questions focus on organic chemistry but enthalpy questions can be applied to an inorganic reaction.

(a) Oxygen is an element in its standard state ✓

(b) $2NaNO_3(s) \rightarrow 2NaNO_2(s) + O_2(g)$

When using enthalpies of formation, the expression below is used:

$\Delta_r H^{\ominus} = \sum \Delta_f H^{\ominus}(\text{products}) - \sum \Delta_f H^{\ominus}(\text{reactants})$ ✓

$\Delta_r H^{\ominus} = 2(-359.4) - 2(-466.7)$ ✓

$= +214.6\,\text{kJ mol}^{-1}$ ✓

ⓔ This reaction is endothermic overall, as you would expect a thermal decomposition to be. Remember to include the sign (+ or –) in front of the enthalpy change value, as leaving this out can cost you a mark.

Question 3

Propane gas burns in oxygen according to the equation:

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$$

The mean bond enthalpies are given in Table 5.

Bond	Mean bond enthalpy (kJ mol^{-1})
C–H	412
C–C	348
O–H	463
O=O	496
C=O	803

Table 5

Which one of the following is the standard enthalpy change of combustion of propene?

A **$-198\,\text{kJ mol}^{-1}$**

B **$-2050\,\text{kJ mol}^{-1}$**

C **$-2398\,\text{kJ mol}^{-1}$**

D **$-4034\,\text{kJ mol}^{-1}$**

Answer is B ✓

ⓔ The total enthalpy required to break the bonds, based on the main equation given is: 2 × 348 + 8 × 412 + 5 × 496 = 6472 kJ. The energy released when bonds form, based on the main equation is: 6 × 803 + 8 × 463 = 8522 kJ. The enthalpy change in the equation is +6472 – 8522 = –2050 kJ. The distractors are: A, where 4 moles of O–H bonds are used; C, where only 1 mole of C–C bond is included; and D, where only one O=O bond is broken, as opposed to five.

Kinetics

Question 1

What label is placed on a vertical axis of a distribution of molecular energies?

A energy

B number of molecules

C frequency

D enthalpy

Answer is B ✓

e The vertical axis is number of molecules. Energy is the horizontal axis and enthalpy would also be a distractor, as enthalpy level diagrams are also used in kinetics.

Question 2

For a gaseous reaction:

$$A(g) + 3B(g) \rightleftharpoons 2C(g) \quad \Delta H = -92\,kJ\,mol^{-1}$$

Figure 1 shows the distribution of molecular energies in the reaction mixture at 450 °C.

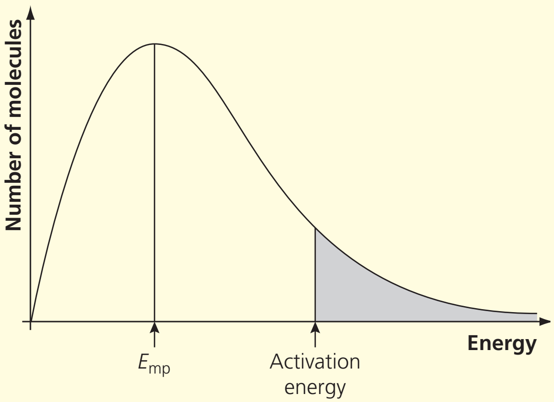

Figure 1

(a) **(i)** Sketch on the diagram the distribution of molecular energies at 500°C. (1 mark)

(ii) Explain, using Figure 1, why the rate of reaction would be faster at 500°C. (2 marks)

(iii) Explain how the yield of C is affected by increasing the temperature to 500°C. (2 marks)

(b) Suggest why a high pressure is used. (2 marks)

(c) Explain, using Figure 1, how a catalyst increases the rate of reaction. (2 marks)

(d) State the effect, if any, on the most probable energy (E_{mp}) of increasing the concentration of A and B. (1 mark)