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Content Guidance

Questions & Answers

Topic 5 Formulae, equations and amounts of substance

The abilities to calculate formulae from data, write correct formulae, balance equations and perform quantitative calculations are fundamental to the whole study of chemistry. This topic introduces these ideas, and its content could be examined in any of the papers.

The ability to lay out calculations in a comprehensible manner depends on:

- knowing what you are doing and not being reliant on rote learning of formulae
- realising that calculations need linking words and phrases to make them readable
- the correct use of units *throughout the calculation*

Using units throughout a calculation is advantageous. It means that you are less likely to get calculations wrong because you are more aware of what you are doing. Some of the advantages are:

- an awareness that equations are not merely symbols, but express relationships between physical quantities
- a check on whether the equations used are in fact correct, because of the in-built check on the units of the answer
- a gradual awareness of what sort of magnitude of answer is reasonable in a given set of circumstances

Amount of substance and the Avogadro constant

In chemistry, the term *amount* has a technical meaning. It refers to the number of moles of substance being considered.

A **mole** is that amount of substance that contains the same number of entities (molecules, ions, atoms) as there are atoms in exactly 0.012 kg (12 g) of the isotope ^{12}C. The entities concerned must also be specified.

The number of entities in a mole of substance is called the **Avogadro constant**, N_A. Its value is $6.02214179 \times 10^{23}\,mol^{-1}$.

The mole is used because chemistry takes place between particles (molecules, ions or atoms). However, the most convenient way of measuring materials in the laboratory is to weigh them. The Avogadro constant, together with the idea of relative molecular mass, provides the necessary link. Water, H_2O, has a relative molecular mass of 18.0. Since 12 g of ^{12}C contains (by definition) N_A carbon atoms, it follows that 18 g of water contains N_A water molecules, since every molecule has a mass 18.0/12 times that of a ^{12}C atom. In fact, for any molecular substance, its relative molecular mass, in grams, contains N_A molecules of that substance. For an ionic substance, its formula mass, in grams, has N_A formula units. This enables reacting masses to be calculated (see page 46).

Exam tip

The number of entities = number of moles × 6.02×10^{23}.

Knowledge check 29

Calculate the number of methane molecules in 0.125 mol of methane.

Exam tip

For an ionic solid, such as NaCl, there are 6.02×10^{23} Na^+ ions and 6.02×10^{23} Cl^- ions per mole. For $CaCl_2$ there are 6.02×10^{23} Ca^{2+} ions and $2 \times 6.02 \times 10^{23}$ Cl^- ions per mole.

Knowledge check 30

Calculate the *total* number of ions in 0.125 mol of aluminium sulfate, $Al_2(SO_4)_3$.

Exam tip

One mole of a substance equals its relative molecular mass in grams.

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Molar mass is the mass (in grams) of a substance that contains N_A molecules or, if ionic, N_A formula units, of the substance. Its units are $g\,mol^{-1}$ and it is numerically the same as the relative molecular (formula) mass of the substance.

Empirical and molecular formulae

The empirical formula of a compound is its formula in its lowest terms — the simplest whole number ratio of atoms in the formula. Therefore, CH_2 is the empirical formula of any compound C_nH_{2n}, i.e. alkenes, cycloalkanes and poly(alkenes).

The calculation steps give you:

- the moles of each atom
- the ratio of moles of each atom

Example 1

A compound contains 73.47% carbon, 10.20% hydrogen and the remainder is oxygen. The relative molecular mass is 98. Find the empirical and molecular formulae of the compound.

Answer

Atom	Divide by A_r (= moles)	Divide by smallest (= ratio of moles)	Ratio of atoms
Carbon	$\frac{73.47}{12.0} = 6.1225$	$\frac{6.1225}{1.020} = 6$	6
Hydrogen	$\frac{10.20}{1.0} = 10.20$	$\frac{10.20}{1.020} = 10$	10
Oxygen	$\frac{16.33}{16.0} = 1.020$	$\frac{1.020}{1.020} = 1$	1

The compound has the empirical formula $C_6H_{10}O$. The mass of this is:

$$(6 \times 12) + (10 \times 1) + 16 = 98$$

So the empirical formula is also the molecular formula.

Exam tip

If the compound contains oxygen, the mass of oxygen has to be calculated by subtracting the masses of hydrogen and carbon from the mass of the compound.

Example 2

2.4 g of a compound containing carbon, hydrogen and oxygen only was burnt and produced 5.28 g of carbon dioxide and 2.88 g of water. Calculate the moles of carbon dioxide and water and hence find the empirical formula of the compound.

→

Knowledge check 31

What is the mass of 1 mol of (a) methane, CH_4 and (b) sodium chloride, NaCl?

Exam tip

You must know the relationships:

$$\text{moles} = \frac{\text{mass}}{\text{molar mass}}$$

$$\text{mass} = \text{moles} \times \text{molar mass}$$

Knowledge check 32

Calculate the number of moles in (a) 2.0 g of methane, CH_4 and (b) 2.0 g of sodium chloride, NaCl.

Knowledge check 33

What is the mass of 0.12 mol of sodium hydroxide?

Exam tip

When you use the periodic table, you must be careful to use atomic masses, not atomic numbers. For example, carbon is 12.0 not 6.

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Student answer

(a) It is the number of protons in one atom of the element. ✓

(b) B ✓

ⓔ The 2⁻ ion has two more electrons than protons.

(c) (i) $X^{2+}(g) - e \rightarrow X^{3+}$ ✓

ⓔ You may write – e on the left or + e on the right.

(ii) C ✓

ⓔ There is a big jump between the fifth and sixth values, so there are five outer electrons.

(iii) In the first ionisation energy the electron is being removed from a neutral atom, whereas in the second it is being removed from a positive ion. ✓ So there is greater attraction between the electron leaving and the already 1+ ion ✓ and so more energy is needed.

(d) B ✓

ⓔ These all have the same electronic configuration as neon. The ions in D have the same number of electrons in their outer orbit.

ⓔ **Total score: 7/7 marks**

Question 2

(a) **When a sample of copper is analysed using a mass spectrometer, its atoms are ionised, accelerated and then separated according to their mass/charge (*m*/*z*) ratio.**

(i) **Explain how the atoms of the sample are ionised.** (2 marks)

(ii) **State how the resulting ions are accelerated.** (1 mark)

(iii) **State how the ions are separated according to their *m*/*z* values.** (1 mark)

(b) **For a particular sample of copper, two peaks were obtained in the mass spectrum, showing an abundance of 69.10% at *m*/*z* 63, and 30.90% at *m*/*z* 65.**

(i) **Give the formula of the species responsible for the peak at *m*/*z* 65.** (1 mark)

ⓔ A perfect answer would include the atomic number, the mass number and any charge on the species.

(ii) **State why two peaks, at *m*/*z* values of 63 and 65, were obtained in the mass spectrum, but no peak is found at an *m*/*z* value of 64.** (1 mark)

(iii) **Calculate the relative atomic mass of this sample of copper to three significant figures, using the data given above.** (2 marks)

(Total: 8 marks)

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Student answer

(a) (i) Fast-moving *or* energetic electrons strike the atoms, ✓ removing electrons from the sample atoms, and forming positive ions ✓.

e The copper sample would be on a heated probe; although the vapour pressure of copper is very small, the number of atoms volatilised at the extremely low pressure in the mass spectrometer is large enough to be detected.

(ii) In an electric *or* electrostatic field ✓

(iii) By a magnetic field ✓

(b) (i) ${}^{65}_{29}Cu^{+}$ ✓

e Many students forget to put the essential positive charge when giving the formula of an ion detected by a mass spectrometer. ${}^{65}Cu^{+}$ would be accepted.

(ii) Because naturally occurring copper contains two isotopes of mass 63 and 65. ✓

(iii) relative atomic mass $= \dfrac{(63 \times 69.10) + (65 \times 30.90)}{69.10 + 30.90} = 63.6$ ✓✓

e The question asks for *three* significant figures. If you give 63.618 or 63.62 you will not score the mark. This is a silly way to lose marks.

e **Total score: 8/8 marks**

Question 3

(a) **Explain the following observations in terms of the intermolecular forces present:**

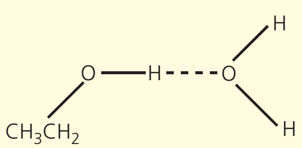
(i) **Ethanol has a much higher boiling temperature (352 K) than propane (231 K), even though the molecules have the same number of electrons.** (4 marks)

e You must mention all the intermolecular forces involved.

(ii) **Ethanol is less polar than chloroethane, but ethanol is soluble in water whereas chloroethane is not.** (4 marks)

(b) **Which of A–D represents most accurately the hydrogen bonding that occurs between ethanol and water?** (1 mark)

A



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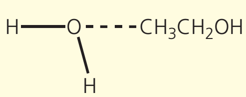

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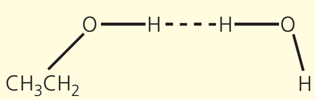

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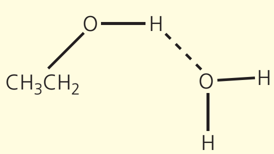

(Total: 9 marks)