

### WJEC (Eduqas) Chemistry A-level Core Topic 1.3 - Chemical Calculations

Flashcards

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## What does the term relative atomic mass mean?







What does the term relative atomic mass mean?

The average mass of one atom of an element compared to 1/12th the mass of an atom of carbon-12.







### What does the term relative formula mass mean?







What does the term relative formula mass mean?

The weighted average of the masses of the formula units compared to 1/12th the mass of an atom of carbon-12.







## What does the term relative molecular mass mean?







What does the term relative molecular mass mean?

The weighted average of the masses of the molecules compared to 1/12th the mass of an atom of carbon-12.







### What does the term relative isotopic mass mean?







What does the term relative isotopic mass mean?

# The mass of one atom of an isotope compared to 1/12th the mass of an atom of carbon-12.







### What is mass spectrometry?







#### What is mass spectrometry?

Mass spectrometry is a type of analytical technique which measures the mass to charge ratio of ions. It also measures how abundant each ion is so it can be used to calculate the relative atomic mass.







# Explain the five stages of TOF mass spectrometry







#### Explain the five stages of TOF mass spectrometry

- 1. Ionisation vapourised sample is injected into the mass spectrometer where it is ionised.
- 2. Acceleration the positively charged ions are accelerated towards a negatively charged detection plate.
- 3. Ion drift the ions are deflected into a curved path with a magnetic field.
- 4. Detection the positive ions are detected by hitting a negatively charged plate, where they gain an electron, producing a current. The greater the current, the greater the abundance.
- 5. Analysis the relative abundance of each isotope are compared. Relevant calculations are made.







## Use the graph to calculate the relative atomic mass





#### Use the graph to calculate the relative atomic mass





### How can you use a mass spectrum to deduce the relative molecular mass of a sample of a compound?







How can you use a mass spectrum to deduce the relative molecular mass of a sample of a compound?

The peak with the highest m/z value (the molecular ion peak,  $M^+$ ) is caused by the whole molecule, therefore m/z value = molecular mass.





Chlorine has two possible isotopes, Cl<sup>35</sup> with a 75% abundance and Cl<sup>37</sup> with a 25% abundance. Predict what the mass spectrum would look like for the diatomic molecule







#### Chlorine has two possible isotopes, Cl<sup>35</sup> with a 75% abundance and Cl<sup>37</sup> with a 25% abundance. Predict what the mass spectrum would look like for the diatomic molecule elative abundance Possible combinations of the $Cl_2^+$ : 35+35=70 35+37=72 37+37=74 The 70:72:74 is in the ratio 9:6:1. 222 332 m/z Some fragmentation occurs so there are also peaks at m/z 35 and 37. www.pmt.education





### Define empirical formula







#### Define empirical formula

# The simplest whole number ratio of atoms of each element in a compound.







### Define molecular formula







#### Define molecular formula

# The actual number of atoms of each element present in a compound.







### What is the empirical formula of $Fe_2O_4$ ?







### What is the empirical formula for $Fe_2O_4$ ?

FeO<sub>2</sub>







# A molecule has the empirical formula $C_4H_3O_2$ and a relative molecular mass of 166. What is the molecular formula?







A molecule has the empirical formula  $C_4H_3O_2$  and a relative molecular mass of 166. What is the molecular formula?

Empirical mass = 4(12) + 3(1) + 2(16) = 83

Relative molecular mass = 166

Compare molecular mass with empirical mass = 166 / 83 = 2

So the molecular formula is double the empirical formula:  $C_8H_6O_2$ 







### Define the Avogadro constant







#### Define the Avogadro constant

# The number of particles in one mole of a substance. This is $6.02 \times 10^{23}$ particles.







# What is the equation linking Avogadro's constant to moles?







What is the equation linking Avogadro's constant to moles?

Number of particles/atoms/ions =

Moles x Avogadro's constant







# There are 4.816 x 10<sup>24</sup> atoms of iron in a sample. How many moles of iron are in the sample?







#### There are $4.816 \times 10^{24}$ atoms of iron in a sample. How many moles of iron are in the sample?

Avogadro's constant =  $6.02 \times 10^{23} \text{ mol}^{-1}$ 

Moles = number of atoms ÷ Avogadro's constant

$$= (4.816 \times 10^{24}) \div (6.02 \times 10^{23})$$

= 8 mol of Fe







### Define molar mass







#### Define molar mass

# The mass per mole of a substance, measured in g mol<sup>-1</sup>.







## What is the equation that links moles to mass?






#### What is the equation that links moles to mass?

Moles =

### Mass (g) x Relative atomic mass







### **Define concentration**







#### Define concentration

#### The amount of moles per unit volume.







# How can concentration be calculated in g/dm<sup>3</sup>?







How can concentration be calculated in g/dm<sup>3</sup>?

## Concentration (g/dm<sup>3</sup>) = Mass (g) / Volume (dm<sup>3</sup>)







# How can concentration be calculated in mol/dm<sup>3</sup>?







How can concentration be calculated in mol/dm<sup>3</sup>?

### Concentration (mol/dm<sup>3</sup>) =

### Moles / Volume (dm<sup>3</sup>)







# 5.00 g of NaCl is dissolved in 25 cm<sup>3</sup> of water. Calculate the concentration of the solution in mol/dm<sup>3</sup>.







5.00 g of NaCl is dissolved in 25 cm<sup>3</sup> of water. Calculate the concentration of the solution in mol/dm<sup>3</sup>.

Volume in 
$$dm^3 = 25 / 1000 = 0.025$$

Concentration in mol/dm<sup>3</sup> = 0.0855 / 0.025

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# What is the molar volume of any gas at room temperature and pressure?







### What is the molar volume of any gas at room temperature and pressure?

24 dm<sup>3</sup>







### What is RTP?







#### What is RTP?

### Room temperature and pressure:

- 20°C
- 1 atmosphere







# What equation links molar volume at RTP and moles?







## What equation links molar volume at RTP and moles?

### Volume of gas at RTP ( $dm^3$ ) = moles x 24







# How many moles of oxygen are in 72 dm<sup>3</sup> at RTP?







#### How many moles of oxygen are in 72 dm<sup>3</sup> at RTP?

# Moles = volume / 24= 72 / 24= 3 moles







### How is the molar volume at a given pressure affected if temperature is increased?







How is the molar volume at a given pressure affected if temperature is increased?

An increase in temperature reduces the molar volume at a given temperature.







### How is the molar volume at a given temperature affected if pressure is increased?







How is the molar volume at a given temperature affected if pressure is increased?

An increase in pressure will mean the maximum molar volume reduces. Up to this maximum, increasing the pressure will increase the molar volume.







### What is the ideal gas law?







#### What is the ideal gas law?

### pV = nRT

- p pressure (Pa)
- V volume  $(m^3)$
- n number of moles
- R gas constant (8.31 J K<sup>-1</sup>mol<sup>-1</sup>)
- T temperature (K)





### At a temperature of 55.0 °C and a pressure of 275 kPa, a gas occupies a volume of 1.10 dm<sup>3</sup>. How many moles of the gas are present? The gas constant is 8.31 J K<sup>-1</sup>mol<sup>-1</sup>.

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At a temperature of 55.0  $^{\circ}$ C and a pressure of 275 kPa, a gas occupies a volume of 1.10 dm<sup>3</sup>. How many moles of the gas are present? The gas constant is 8.31 J K<sup>-1</sup>mol<sup>-1</sup>.

pV = nRT

- 275 kPa in Pa is 275000
  Pa
- 55.0 °C in K is 328 K
- 1.10 dm<sup>3</sup> is 0.001 m<sup>3</sup>

n=(pV)/(RT)

n=(275000 x 0.001)/(8.31 x 328)

n= 0.10 moles

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### How can percentage yield be calculated?







#### How can percentage yield be calculated?

### Percentage yield =

### (Actual yield + Theoretical yield) x 100







### What is the percentage yield of $NH_3$ if 40.5 g of $NH_3$ is produced from 20.0 mol $H_2$ and excess $N_2$ ?







What is the percentage yield of  $NH_3$  if 40.5 g of  $NH_3$  is produced from 20.0 mol  $H_2$  and excess  $N_2$ ?

Equation: 
$$N_2 + 3H_2 \rightarrow 2NH_3$$

- Moles of ammonia = 20/1.5 = 13.3 moles
- Mass of ammonia =  $13.3 \times (14+1+1+1) = 227 \text{ g}$

Percentage yield = (40.5/227) x 100 = 17.9%





# Why might the actual yield of product be less than expected?







Why might the actual yield of product be less than expected?

- Incomplete reaction
- Unwanted side reactions
- Practical losses, for example some solid may get lost when being transferred between beakers





### What is the atom economy of a reaction?







What is the atom economy of a reaction?

Atom economy is a measure of the efficiency of the reaction. It looks at the amount of reactants that get turned into useful products.







### How can atom economy be calculated?







#### How can atom economy be calculated?

#### Atom economy=

#### (Mr of desired product ÷ total Mr of reactants) x 100







# Fill in the gap: 'The \_\_\_\_\_ the atom economy, the more sustainable and efficient the process'






## Fill in the gap: 'The \_\_\_\_\_ the atom economy, the more sustainable and efficient the process'

#### Higher







# How can percentage error be calculated?







#### How can percentage error be calculated?

#### % error = <u>absolute uncertainty</u> x 100 calculated value







### A titre volume is recorded as 11.30 cm<sup>3</sup>. The accuracy of the burette is ±0.05cm<sup>3</sup>. Calculate the maximum percentage error.







A titre volume is recorded as  $11.30 \text{ cm}^3$ . The accuracy of the burette is  $\pm 0.05 \text{ cm}^3$ . Calculate the maximum percentage error.

### % error = <u>absolute uncertainty</u> x 100 calculated value

#### $(0.05 \div 11.30) \times 100 = 0.442\%$



