

WJEC (Wales) Chemistry A-level

Topic 1.3 - Chemical Calculations

Flashcards

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What does the term relative atomic mass mean?



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The average mass of one atom of an element compared to $1/12^{\text{th}}$ 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 $1/12^{\text{th}}$ 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 $1/12^{\text{th}}$ 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 $1/12^{\text{th}}$ 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

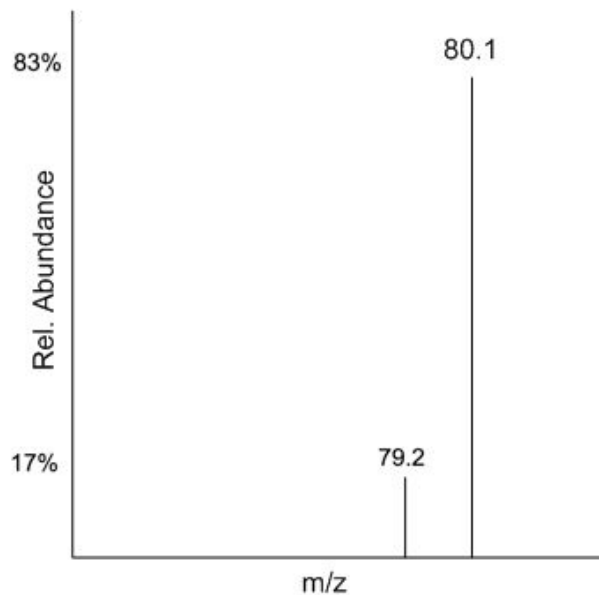


Explain the five stages of TOF mass spectrometry

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.



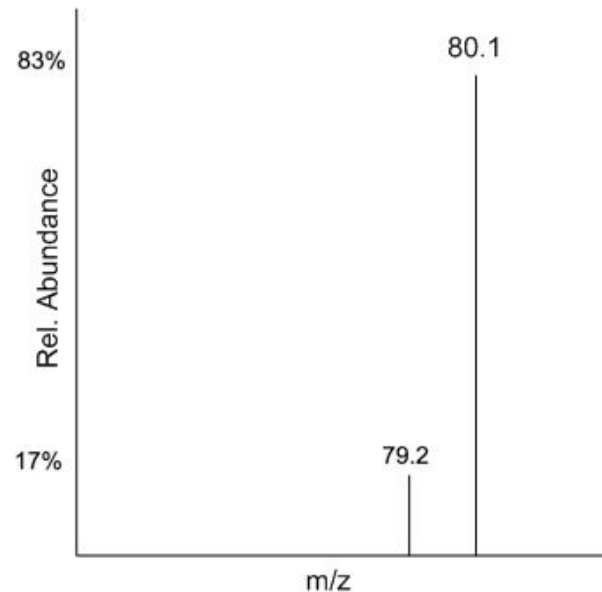
Use the graph to calculate the relative atomic mass



Use the graph to calculate the relative atomic mass

$$[(79.2 \times 17) + (80.1 \times 83)] \div 100$$

$$= 79.95 \text{ g mol}^{-1}$$



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^{35} with a 75% abundance and Cl^{37} with a 25% abundance. Predict what the mass spectrum would look like for the diatomic molecule



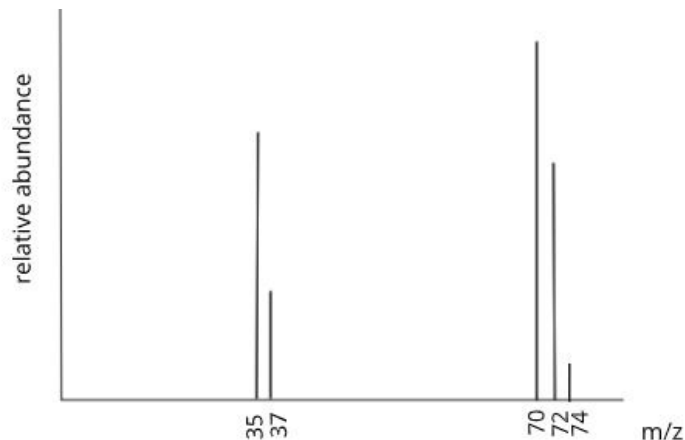
Chlorine has two possible isotopes, Cl^{35} with a 75% abundance and Cl^{37} with a 25% abundance. Predict what the mass spectrum would look like for the diatomic molecule

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.

Some fragmentation occurs so there are also peaks at m/z 35 and 37.



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 ?



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?

$$\text{Empirical mass} = 4(12) + 3(1) + 2(16) = 83$$

$$\text{Relative molecular mass} = 166$$

$$\text{Compare molecular mass with empirical mass} = 166 / 83 = 2$$

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 6.02×10^{23} particles.



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



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Number of particles =

Moles x Avogadro's constant



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



There are 4.816×10^{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 \div Avogadro's constant

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

$$= 8 \text{ mol of Fe}$$



Define molar mass



Define molar mass

The mass per mole of a substance,
measured in g mol^{-1} .



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^3 ?



How can concentration be calculated in g/dm^3 ?

Concentration (g/dm^3) =

Mass (g) / Volume (dm^3)



How can concentration be calculated in
 mol/dm^3 ?



How can concentration be calculated in mol/dm^3 ?

Concentration (mol/dm^3) =

Moles / Volume (dm^3)



5.00 g of NaCl is dissolved in 25 cm³ of water. Calculate the concentration of the solution in mol/dm³.



5.00 g of NaCl is dissolved in 25 cm³ of water.
Calculate the concentration of the solution in
mol/dm³.

$$\text{Moles of NaCl} = 5 / 58.5 = 0.0855$$

$$\text{Volume in dm}^3 = 25 / 1000 = 0.025$$

$$\text{Concentration in mol/dm}^3 = 0.0855 / 0.025 = 3.42 \text{ mol/dm}^3$$



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 dm³



What is RTP?



What is RTP?

Room temperature and pressure:

- 20°C
- 1 atmosphere



What equation links molar volume at
RTP to moles?



What equation links molar volume at RTP to moles?

Volume of gas at RTP (dm^3) = moles \times 24



How many moles of oxygen are in
 72 dm^3 at RTP?



How many moles of oxygen are in 72 dm^3 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 ($8.31 \text{ J K}^{-1}\text{mol}^{-1}$)

T - temperature (K)



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



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

$$pV = nRT$$

- 275 kPa is 275000 Pa
- $55.0\text{ }^{\circ}\text{C}$ is 328 K
- 1.10 dm^3 is 0.001 m^3

Therefore,

$$n = (pV)/(RT)$$

$$n = (275000 \times 0.001)/(8.31 \times 328)$$

$$n = 0.10\text{ moles}$$



How can percentage yield be calculated?



How can percentage yield be calculated?

Percentage yield =

$(\text{Actual yield} \div \text{Theoretical yield}) \times 100$



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 ?



Moles of ammonia = $20/1.5 = 13.3$ moles

Mass of ammonia = $13.3 \times (14+1+1+1) = 227$ g

Percentage yield = $(40.5/227) \times 100 = 17.9\%$



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 =

$(\text{Mr of desired product} \div \text{total Mr of reactants}) \times 100$



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?

$$\% \text{ error} = \frac{\text{absolute uncertainty}}{\text{calculated value}} \times 100$$



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



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

$$\% \text{ error} = \frac{\text{absolute uncertainty}}{\text{calculated value}} \times 100$$

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

