



Mass Spectrometry

A Level



Mass spectrometry is a technique for studying chemical substances. High resolution mass spectrometry allows us to determine relative atomic or molecular masses to a high degree of precision. Some forms of mass spectrometry can also provide structural information which is useful for structure determination.

Part A Electron ionisation

A mass spectrometer relies on the presence of ions, which it is able to separate by their mass to charge ratio. However, many samples we wish to study are neutral. The instrument therefore needs to use an ionisation technique to form these ions within the sample. We will first consider **electron ionisation (EI)**. This involves firing high energy electrons at the vaporised sample in order to remove electrons.

Which of the following equations is an accurate description of this electron ionisation process:

- ☐ $X(g) \longrightarrow X^{-}(g) + e^{-}$
- ☐ $X^{+}(g) + e^{-} \longrightarrow X(g)$
- ☐ $X(g) + e^{-} \longrightarrow X^{-}(g)$
- ☐ $X(g) + e^{-} \longrightarrow X^{+}(g) + 2e^{-}$

Part B Fragmentation

Electron ionisation is a hard ionisation technique, which means it often results in fragmentation of the molecular ion formed initially. As a consequence, when applied to large molecules, the mass spectrum often contains many features corresponding to these lighter ions. This can be helpful for structure determination: for a given molecular structure, we can predict likely ways in which the molecular ion might fragment (e.g. through particular bonds breaking) and check whether this is consistent with the spectrum. That said, some of the fragmentations are far more complex than simple bond breaking and involve rearrangements. This can make it difficult to account for the formation of certain ions even if we confidently know the molecular structure already.

A student was thinking about fragmentation in mass spectrometers and hypothesised that if they saw a fragment feature 15 mass units lighter than the molecular ion, they should also see a feature due to an ion with mass 15. However, consulting some real spectra, they found that it is in fact common not to see ion pairs that “complement” each other like this. By carefully considering a single, simple fragmentation process occurring on a molecular ion, suggest why this might be.

Part C Electrospray ionisation

A softer ionisation technique, resulting in far less fragmentation than electron ionisation, is **electrospray ionisation**. There are a number of variations of this, but in one type, the neutral atom or molecule bonds to a proton (hydrogen ion).

Select the correct equation describing this process for sodium:

- ☐ $\text{Na(g)} + \text{H}^-(\text{g}) \longrightarrow [\text{Na} + \text{H}]^-(\text{g})$
 - ☐ $\text{Na(g)} + \text{H}^+(\text{g}) \longrightarrow \text{Mg}^+(\text{g})$
 - ☐ $\text{Na(g)} + \text{H}^-(\text{g}) \longrightarrow \text{Ne}^-(\text{g})$
 - ☐ $\text{Na(g)} + \text{H}^+(\text{g}) \longrightarrow \text{Ne}^+(\text{g})$
 - ☐ $\text{Na(g)} + \text{H}^-(\text{g}) \longrightarrow \text{Mg}^-(\text{g})$
 - ☐ $\text{Na(g)} + \text{H}^+(\text{g}) \longrightarrow [\text{Na} + \text{H}]^+(\text{g})$
-

Part D Time-of-flight expression

In a time-of-flight (TOF) mass spectrometer, the ions formed are accelerated through a potential so that all singly-charged ions have the same kinetic energy, E . These ions then travel along a flight tube of length d before reaching the detector. The delay is a function of the mass of a given ion, m .

Derive a formula for the time it takes an ion to travel along the flight tube (the time of flight) as a function of E , d and m . Assume that all quantities are provided in SI units, so your formula does not need to take into account any conversion factors.

The following symbols may be useful: E , d , m

Part E Calculating molecular mass

Based on the above formula, ions of different mass take different amounts of time to travel through the spectrometer. Calculate, in kg, the mass of an ion X^+ that takes 7.55×10^{-6} s to travel through the 2.00 m drift region, assuming it was previously accelerated to a kinetic energy of 5.83×10^{-15} J.

Part F Converting to atomic mass units

Convert the above mass of X^+ in kg to atomic mass units (amu) in which you more typically express the mass of atoms, molecules and ions in chemistry.

Part G Electron mass

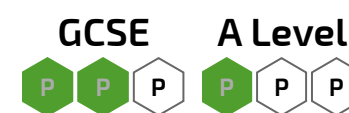
To obtain the mass of the neutral species, X , we would actually need to add on the mass of an electron. Why is this not a particularly meaningful calculation for the above quantities?



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Essential Pre-Uni Chemistry A2.3



Assume that the mass of an isotope in amu to 3 significant figures is equal to its mass number.

Magnesium has the following natural isotopes: ^{24}Mg 78.6%; ^{25}Mg 10.1%; ^{26}Mg 11.3%.

Calculate the relative atomic mass of magnesium. Give your answer to 3 significant figures.

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Essential Pre-Uni Chemistry A2.5

Assume that the mass of an isotope in amu to 3 s.f. is equal to its mass number.

Complete the table shown below.

Element	A_r	Isotope 1	Isotope 2	Isotope 3	Isotope 4
Bromine	Part A	^{79}Br 50.5%	^{81}Br 49.5%	n/a	n/a
Silver	107.9	Part B ^{107}Ag ? %	Part C ^{109}Ag ? %	n/a	n/a
Cerium	140.2	^{136}Ce 0.2%	^{138}Ce 0.2%	^{140}Ce 88.5%	Part D $^{?}\text{Ce}$ 11.1%

Part A Br

Give the value of A_r for Br to 3 significant figures.

Part B ^{107}Ag

Give the percent abundance of ^{107}Ag to 2 significant figures.

Part C ^{109}Ag

Give the percent abundance of ^{109}Ag to 2 significant figures.

Part D **Ce isotope 4**

What is the mass number of isotope 4 of Ce?

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Essential Pre-Uni Chemistry A2.7



Assume that the mass of an isotope in amu to 3 significant figures is equal to its mass number.

Complete combustion of compound N occurs in a stoichiometric ratio of 1 : 6 with oxygen gas. Complete combustion of 4.2 g of compound N produces 13.2 g of carbon dioxide and 5.4 g of water.

Find the molecular formula of N.

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Combinatorics With Isotopes

Chlorine consists of two isotopes, ^{35}Cl and ^{37}Cl , in the abundance ratio 3:1. Phosphorus is mono-isotopic, ^{31}P .

Apart from the lines due to atomic ions, the mass spectrum of a chloride of phosphorus contains 9 lines arranged in 3 groups:

group	m/z values of lines
A	66, 68
B	101, 103, 105
C	136, 138, 140, 142

Part A Group A ion

Identify the ion responsible for group **A** (do not use isotope labels in your formula).

Part B Group B ion

Identify the ion responsible for group **B** (do not use isotope labels in your formula).

Part C Group C ion

Identify the ion responsible for group **C** (do not use isotope labels in your formula).

Part D Group A abundance ratio

Predict the abundance ratio of the different m/z values within group **A**. Your answer should be in the form $X_1 : X_2$ (no spaces), where X_1 and X_2 are the smallest possible integers, and the ordering is from lowest to highest m/z value.

Part E Group B abundance ratio

Predict the abundance ratio of the different m/z values within group **B**. Your answer should be in the form $X_1 : X_2 : X_3$ (no spaces), where X_1 , X_2 and X_3 are the smallest possible integers, and the ordering is from lowest to highest m/z value.

Part F Group C abundance ratio

Predict the abundance ratio of the different m/z values within group **C**. Your answer should be in the form $X_1 : X_2 : X_3 : X_4$ (no spaces), where X_1 , X_2 , X_3 and X_4 are the smallest possible integers, and the ordering is from lowest to highest m/z value.

Adapted with permission from UCLES, A Level Chemistry, November 1995, Paper 1, Question 2

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Elements Reversal

A Level



Although the elements in Mendeleev's table are primarily arranged by atomic mass, this was not the case with tellurium (Te) and iodine (I). Mendeleev realised that the chemical properties of the elements meant that tellurium had to come before iodine, but the atomic masses did not support this order. He marked the mass of tellurium with a question mark to highlight its suspicious value.

The modern value for the relative atomic mass of tellurium is one of the least precise: 127.60 ± 0.03 . The reason for the uncertainty is that naturally occurring tellurium is a mix of 8 different isotopes whose proportions can vary depending on the sample. In contrast, naturally occurring iodine consists of a single isotope – iodine 127 – and so its relative mass is known to a high degree of precision: 126.904472 ± 0.000003 .

Part A Protons in iodide

State the number of protons in an iodide ion.

Part B Neutrons in iodide

State the number of neutrons in an iodide ion.

Part C Electrons in iodide

State the number of electrons in an iodide ion.

Part D Tellurium-130

The heaviest of the isotopes found in naturally occurring tellurium is tellurium-130 which has a relative mass of 129.906223. Technically, tellurium-130 is very slightly radioactive and if there were none in the naturally occurring element, the relative atomic mass of tellurium would be 126.412449 (which would make it less than iodine).

Calculate the percentage of tellurium-130 present in naturally-occurring tellurium to 4 significant figures.

Adapted with permission from the Cambridge Chemistry Challenge 2019, Question 1

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Essential Pre-Uni Chemistry B7.1



Nitric acid of unknown concentration was added to a burette. 25.00 cm^3 of potassium hydroxide solution at a concentration of 0.100 mol dm^{-3} was transferred to a 250 cm^3 conical flask using a volumetric pipette. A few drops of methyl orange indicator were added to the flask.

Part A Indicator colour

Give the colour of the indicator in the alkaline solution in the flask

- ☐ peach
- ☐ red
- ☐ blue
- ☐ yellow
- ☐ colourless
- ☐ orange

Part B B7.1b

The nitric acid was added to the flask a little at a time until the resulting solution went pink. The whole process was repeated until concordant titres (within 0.10 cm^3) were obtained.

The concentration of nitric acid was found to be 0.0920 mol dm^3 .

Calculate the titre obtained, in cm^3 . Give your answer to 3 significant figures.

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Essential Pre-Uni Chemistry B7.2



2.50 g of an unknown carbonate were dissolved in 100 cm³ of 1.00 mol dm⁻³ hydrochloric acid (an excess). The resulting solution was made up to 250 cm³ in a volumetric flask. 25.00 cm³ aliquots of this solution were titrated against 0.250 mol dm⁻³ sodium hydroxide. Some of the results are shown below. Fill in the gaps in the table (Parts A-D), and then calculate the quantities in Parts E-L to identify the cation (Part M).

Titration	Initial burette reading / cm ³	Final burette reading / cm ³	Titre / cm ³
Rough	0.60	25.10	Part A
1	0.15	Part B	24.10
2	Part C	25.25	24.45
3	1.35	25.45	Part D

Part A Rough, Titre/cm³

Give your answer to 4 significant figures.

Part B 1, Final burette reading/cm³

Give your answer to 4 significant figures.

Part C 2, Initial burette reading/cm³

Give your answer to 2 significant figures.

Part D 3, Titre/cm³

Give your answer to 4 significant figures.

Part E Average concordant titre

Calculate the average concordant titre. Give your answer to 4 significant figures.

Part F Amount of sodium hydroxide

Calculate the amount of sodium hydroxide in that volume. Give your answer to 3 significant figures.

Part G Amount of hydrochloric acid

The amount of hydrochloric acid in each aliquot. Give your answer to 3 significant figures.

Part H Initial amount of HCl

Calculate the initial amount of hydrochloric acid added to the carbonate. Give your answer to 3 significant figures.

Part I Final amount of HCl

Calculate the amount of hydrochloric acid remaining after reaction. Give your answer to 3 significant figures.

Part J Amount of HCl used

Calculate the amount of hydrochloric acid used in reaction with the carbonate. Give your answer to 3 significant figures.

Part K Amount of carbonate

Calculate the amount of carbonate in 2.50 g. Give your answer to 3 significant figures.

Part L Molar mass of carbonate

Calculate the molar mass of the carbonate. Give your answer to 3 significant figures.

Part M Identity of cation

Identify the cation in the carbonate.

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Essential Pre-Uni Chemistry B7.4

A Level



Three students each prepare a standard solution by dissolving 10.6 g of solid from different bottles labelled 'sodium carbonate' in exactly 1 dm^3 of water. They use this standard solution in a titration to determine the exact concentration of a solution of sulfuric acid at approximately 0.1 mol dm^{-3} . They each use a pipette to measure out exactly 25.00 cm^3 of the standard solution into a conical flask, they each use the same indicator and they each carry out their titrations with great care and accuracy.

The volumes of sulfuric acid solution that they each use are listed below. Only student A finds the correct concentration of the sulfuric acid. Student B is within 20 % but student C is so far out that they know something is wrong. Student C asks for help and is reminded that some solids can contain water of crystallisation. Student A uses anhydrous sodium carbonate, but what is x in the formula $\text{Na}_2\text{CO}_3 \cdot x\text{H}_2\text{O}(\text{s})$ for students B and C?

Student A: 23.75 cm^3

Student B: 20.20 cm^3

Student C: 8.80 cm^3

Part A Acid concentration

Calculate the exact concentration of the sulfuric acid. Give your answer to 3 significant figures.

Part B $\text{Na}_2\text{CO}_3 \cdot x\text{H}_2\text{O}(\text{s})$

Find x in $\text{Na}_2\text{CO}_3 \cdot x\text{H}_2\text{O}(\text{s})$ for student B.

Find x in $\text{Na}_2\text{CO}_3 \cdot x\text{H}_2\text{O}(\text{s})$ for student C.

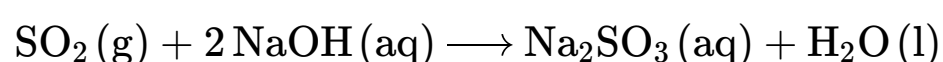


Titrating Sulfur Dioxide



Sulfur dioxide is a by-product of the combustion of coal in power stations. It can react with oxygen and water vapour in the air to form sulfuric acid, H_2SO_4 . This is one of the causes of acid rain.

The amount of sulfur dioxide in the air may be determined by bubbling a sample of the air through sodium hydroxide solution, where it reacts according to the equation below:



The concentration of the unreacted sodium hydroxide can be determined by titration against a standard solution of hydrochloric acid.

1000 dm^3 of air were bubbled through 200 cm^3 of a 1.00 mol dm^{-3} solution of sodium hydroxide. The remaining solution was diluted to 1000 cm^3 with water, and 25.0 cm^3 of this solution was neutralised by 20.4 cm^3 of a 0.100 mol dm^{-3} solution of hydrochloric acid.

Part A H_2SO_4 formation

Construct an overall equation for the formation of sulfuric acid from sulfur dioxide (do not include state symbols). Balance it so as to use the smallest possible integer coefficients.

Part B Neutralisation reaction

Give the (net) ionic equation for the reaction of sodium hydroxide with hydrochloric acid.

Part C Unreacted moles

Find the amount, in moles, of unreacted sodium hydroxide.

Part D Sulfur dioxide moles

Find the amount, in moles, of sulfur dioxide in 1000 dm^3 of air.

Part E Percentage by volume

Hence calculate the percentage by volume of sulfur dioxide in air. (You may assume 1 mol of any gas occupies 24 dm^3 at this temperature and pressure.)

Adapted with permission from OCR, A Level Chemistry, June 1999, General and Physical Paper, Question 3

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