

Chemistry A level Summer Work

This summer work is in three sections:

1. Background Reading and questions on Mass Spectrometry
2. Revision of GCSE calculations and linking these to A level
3. Revision of GCSE bonding and linking this to A level

Please make sure that

1. ALL questions have been completed on paper, clearly showing all your working
2. Notes have been made as evidence of your background reading using the links provided

TASK 1: Mass Spectrometry

Read through the information on a process called mass spectrometry and how it is used. You should also read around this topic using online resources.

Make detailed notes on mass spectrometry including; the processes of electron impact ionisation, electrospray ionisation and how a spectrometer works to determine the mass of an ion.

Student guide: Time of flight mass spectrometry

This guide relates to section 3.1.1.2 of our AS and A-level Chemistry specifications. We have produced it to supplement the specification and the Teaching Notes that are already available. On a separate document we have given you a range of summary questions on the topic with example marking guidance.

Time of flight mass spectrometry

Mass spectrometry is a powerful instrumental method of analysis. It can be used to:

- find the abundance and mass of each isotope in an element allowing us to determine its relative atomic mass
- find the relative molecular mass of substances made of molecules.

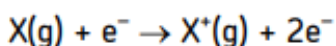
A common form of mass spectrometry is time of flight (ToF) mass spectrometry. In this technique, particles of the substance are ionised to form 1+ ions which are accelerated so that they all have the same kinetic energy. The time taken to travel a fixed distance is then used to find the mass of each ion in the sample.

Stage 1 – Ionisation

The sample can be ionised in a number of ways. Two of these techniques are electron impact and electrospray ionisation (which are simplified here for AS/A level).

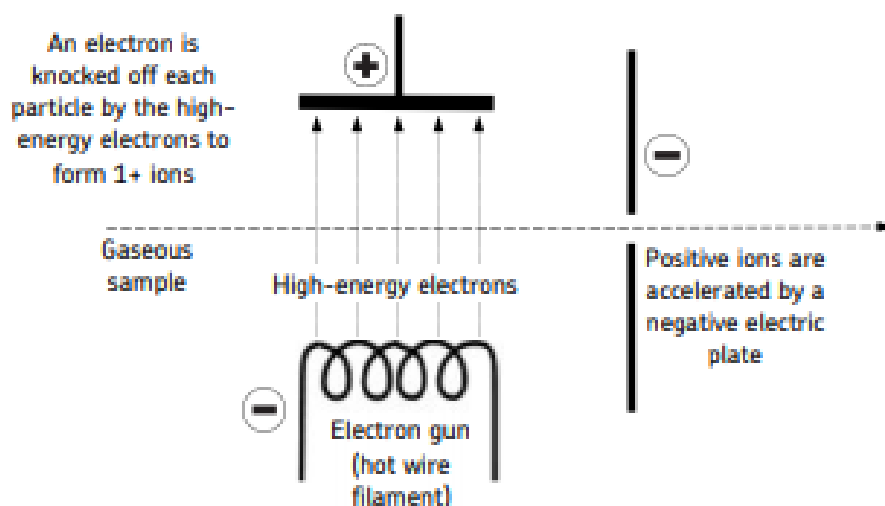
Electron impact (also known as electron ionisation)

The sample being analysed is vaporised and then high energy electrons are fired at it. The high energy electrons come from an 'electron gun' which is a hot wire filament with a current running through it that emits electrons. This usually knocks off one electron from each particle forming a 1+ ion.



(also written as $X(g) \rightarrow X^{+}(g) + e^{-}$)

The 1+ ions are then attracted towards a negative electric plate where they are accelerated.



This technique is used for elements and substances with low formula mass (that can be inorganic or organic molecules). When molecules are ionised in this way, the 1+ ion formed is known as a molecular ion.



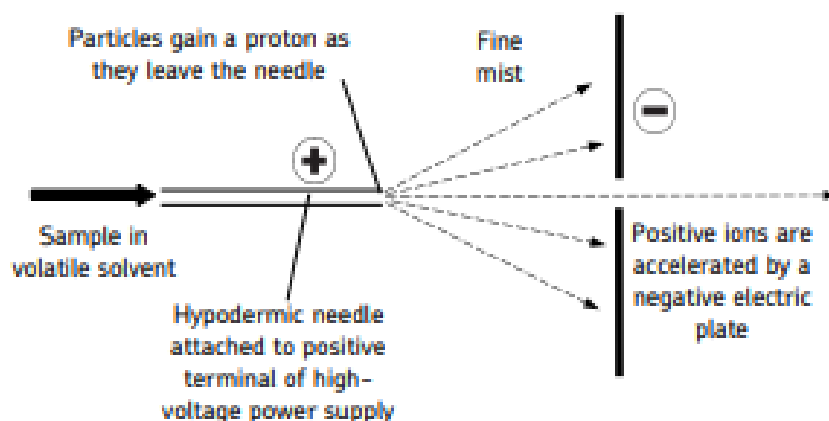
The molecular ion often breaks down into smaller fragments some of which are also detected in the mass spectrum. (Fragmentation of molecular ions is not included on the specification and is only included here as useful background information).

Electrospray ionisation

The sample X is dissolved in a volatile solvent (eg water or methanol) and injected through a fine hypodermic needle to give a fine mist (aerosol). The tip of the needle is attached to the positive terminal of a high-voltage power supply. The particles are ionised by gaining a proton (ie an H^+ ion which is simply one proton) from the solvent as they leave the needle producing XH^+ ions (ions with a single positive charge and a mass of $M_r + 1$).



The solvent evaporates away while the XH^+ ions are attracted towards a negative plate where they are accelerated.



This technique is used for many substances with higher molecular mass including many biological molecules such as proteins. This is known as a 'soft' ionisation technique and fragmentation rarely takes place.

Stage 2 – Acceleration

The positive ions are accelerated using an electric field so that they all have the same kinetic energy.

$$KE = \frac{1}{2}mv^2$$

(students would be given this equation if expected to use it in an exam)

KE = kinetic energy of particle (J)

m = mass of the particle (kg)

v = velocity of the particle ($m\ s^{-1}$)

Therefore, the velocity of each particle is given by: $v = \sqrt{\frac{2KE}{m}}$

Given that all the particles have the same kinetic energy, the velocity of each particle depends on its mass. Lighter particles have a faster velocity, and heavier particles have a slower velocity.

Stage 3 – Flight tube

The positive ions travel through a hole in the negatively charged plate into a tube. The time of flight of each particle through this flight tube depends on its velocity which in turn depends on its mass.

The time of flight along the flight tube is given by the following expression:

$$t = \frac{d}{v}$$

$$t = d\sqrt{\frac{m}{2KE}}$$

(students would be given this equation if expected to use it in an exam)

t = time of flight (s)

d = length of flight tube (m)

v = velocity of the particle (m s^{-1})

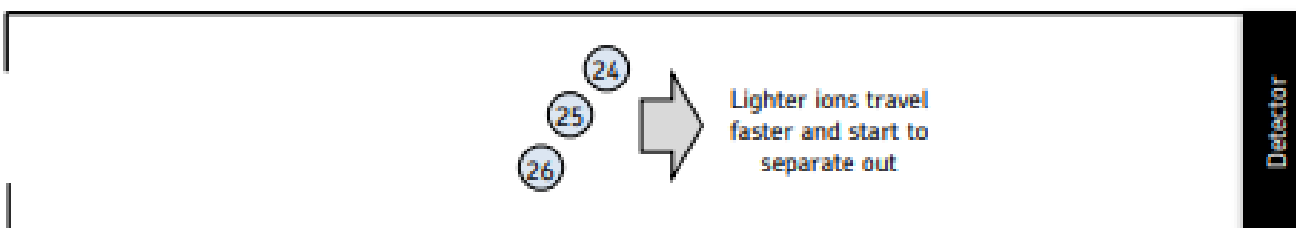
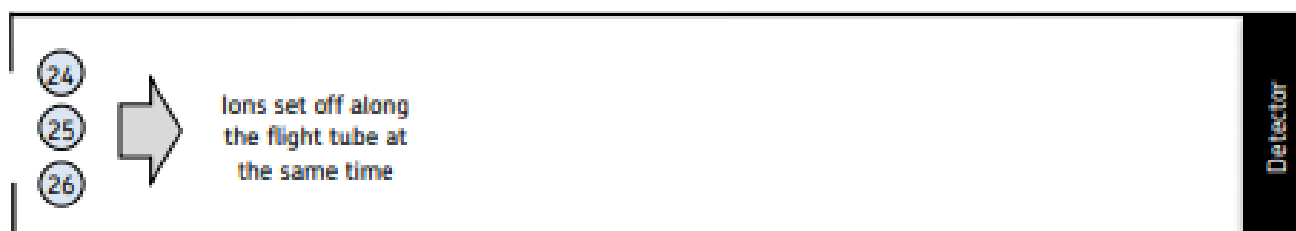
m = mass of the particle (kg)

KE = kinetic energy of particle (J)

This shows that the time of flight is proportional to the square root of the mass of the ions. Therefore lighter ions travel faster and reach the detector in less time than the heavier particles that move slower and take longer to reach the detector.

eg ions of the three isotopes of magnesium ($^{24}\text{Mg}^+$, $^{25}\text{Mg}^+$, $^{26}\text{Mg}^+$) will travel at different speeds through the flight tube and separate, with the lightest ion ($^{24}\text{Mg}^+$) reaching the detector first.

Flight tube



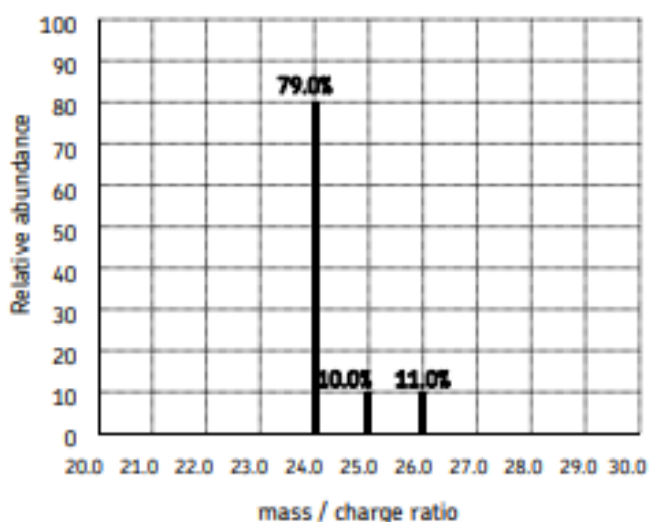
Stage 4 – Detection

The positive ions hit a negatively charged electric plate. When they hit the detector plate, the positive ions are discharged by gaining electrons from the plate. This generates a movement of electrons and hence an electric current that is measured. The size of the current gives a measure of the number of ions hitting the plate.

The mass spectrum

A computer uses the data to produce a mass spectrum. This shows the mass to charge (m/z) ratio and abundance of each ion that reaches the detector. Given that all ions produced by electrospray ionisation and most of the ions by electron ionisation have a 1+ charge, the m/z is effectively the mass of each ion.

In the following example, the mass spectrum of magnesium is shown. Ions with mass to charge ratio 24.0, 25.0 and 26.0 reach the detector. This shows that magnesium is made up of three isotopes: ^{24}Mg , ^{25}Mg and ^{26}Mg .



The relative atomic mass of an element can be found by calculating the mean mass of these isotopes.

$$\text{relative atomic mass } (A_r) = \frac{\text{combined mass of all isotopes}}{\text{combined abundance of all isotopes}}$$

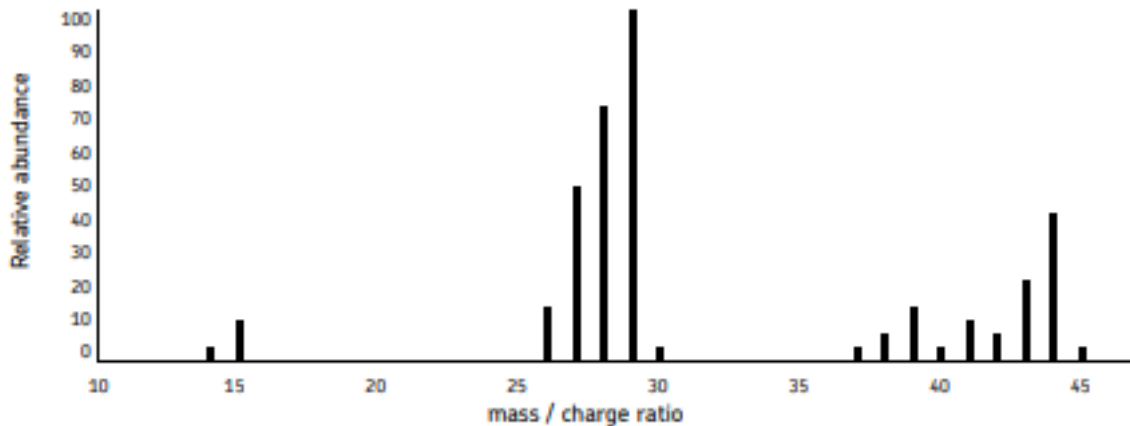
eg for magnesium:

$$\text{relative atomic mass } (A_r) = \frac{(79.0 \times 24.0) + (10.0 \times 25.0) + (11.0 \times 26.0)}{79.0 + 10.0 + 11.0} = 24.3$$

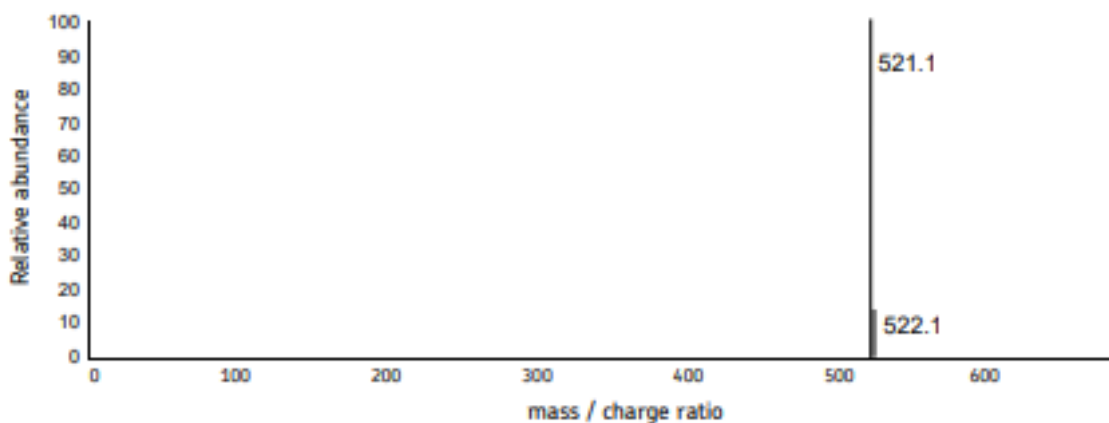
For molecules that are ionised by electron impact, the signal with the greatest m/z value is from the molecular ion and its m/z value gives the relative molecular mass. However, there may be some other small peaks present around the molecular ion peak due to molecular ions that contain different isotopes.

When using electron impact ionisation (but not with electrospray ionisation), there may also be peaks at lower m/z values due to fragments caused by the break up of molecular ion. (Fragmentation of molecular ions is not included on the specification and is only included here as useful background information.)

In the following example, the mass spectrum of propane has been produced following electron impact ionisation. The peak with the greatest m/z is at 44 (apart from a small signal at m/z 45 which is due to molecular ions of propane with one atom of ^2H or ^{13}C). This tells us that the relative molecular mass of propane is 44. Peaks at below m/z 44 are due to the fragmentation of molecular ions.



In this next example, a protein has been analysed by time of flight spectrometry following electrospray ionisation using protonation. The peak at 521.1 is for MH^+ and so the relative molecular mass of the protein is 520.1. The peak at 522.1 is due to MH^+ ions containing one atom of ^{13}C or ^2H .



Answer the following questions in detail

- 1) What happens during electron impact ionisation?
- 2) What type of molecules is this method used with and why?
- 3) Research and write a *brief* description of the new method of forming ions: Electrospray Ionisation
- 4) What type of molecules is this new method suited for use with and why?
- 5) Why is electrospray ionisation considered a soft technique?

Working out Time of Flight (TOF)

Firstly, you can use the method below to work out the velocity of the particles:

The positive ions are accelerated using an electric field so that they all have the same kinetic energy.

$$KE = \frac{1}{2}mv^2$$

(students would be given this equation if expected to use it in an exam)

KE = kinetic energy of particle (J)

m = mass of the particle (kg)

v = velocity of the particle (m s^{-1})

Therefore, the velocity of each particle is given by: $v = \sqrt{\frac{2KE}{m}}$

Given that all the particles have the same kinetic energy, the velocity of each particle depends on its mass. Lighter particles have a faster velocity, and heavier particles have a slower velocity.

Working out Time of Flight (TOF)

Secondly, you use your calculated velocity to work out the time taken for that particle to move through the flight tube:

The positive ions travel through a hole in the negatively charged plate into a tube. The time of flight of each particle through this flight tube depends on its velocity which in turn depends on its mass

$$t = \frac{d}{v}$$

$$t = d\sqrt{\frac{m}{2KE}}$$

(students would be given this equation if expected to use it in an exam)

t = time of flight (s)

d = length of flight tube (m)

v = velocity of the particle (m s^{-1})

m = mass of the particle (kg)

KE = kinetic energy of particle (J)

Complete the exam questions:

(b) Describe how ions are formed in a time of flight (TOF) mass spectrometer.

(2)

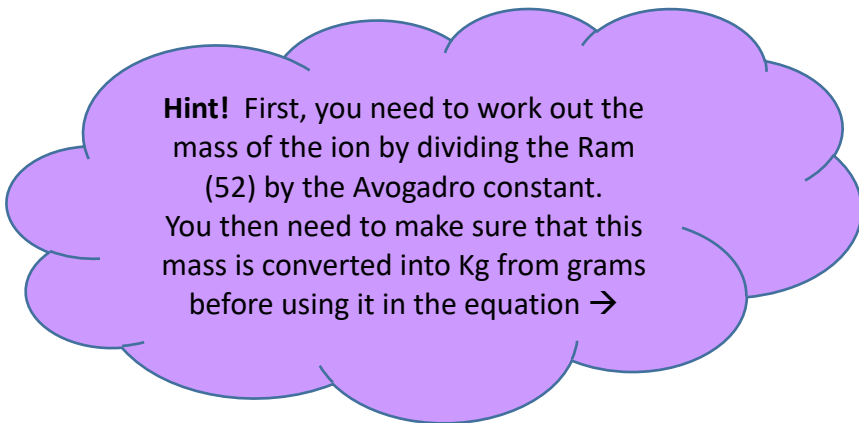
(c) A TOF mass spectrometer can be used to determine the relative molecular mass of molecular substances.

Explain why it is necessary to ionise molecules when measuring their mass in a TOF mass spectrometer.

(a) Explain how ions are accelerated, detected and have their abundance determined in a time of flight (TOF) mass spectrometer.

(3)

TOF Mass Spec Calculation:



(1)

- (c) In a TOF mass spectrometer the kinetic energy (KE) of a $^{52}\text{Cr}^+$ ion was $1.269 \times 10^{-13} \text{ J}$

Calculate the velocity of the ion using the equation.

$$\text{KE} = \frac{1}{2}mv^2$$

(m = mass/kg and v = velocity/ ms^{-1})

(2)

Task 2: Calculations consolidation

Now you need to spend some time revising the following GCSE calculations before trying the next A level exam questions:

- **RFM**
- **Calculating moles in solids from mass**
- **Calculating percentage by mass**
- **The Avogadro Constant**

The following information may help you, but you should be reading through your GCSE work too and doing some research to find out answers that you may not already know.

The Avogadro Constant

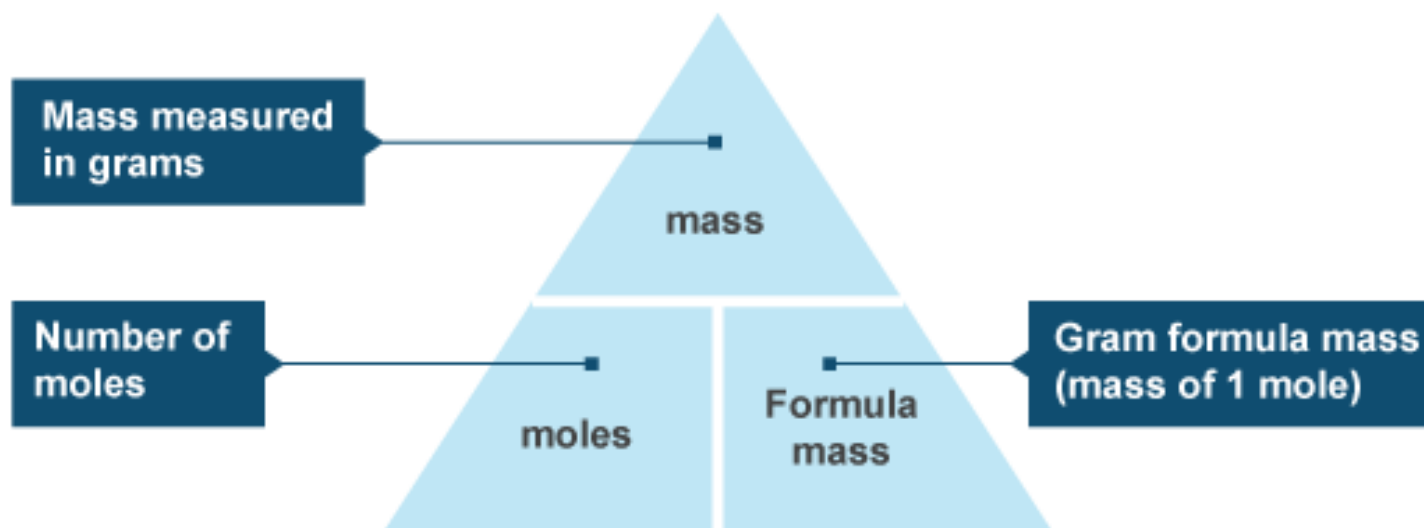
- One mole of a substance is its **gram formula mass (GFM)** e.g. one mole of carbon will weigh 12g (as stated on the Periodic Table)
- One mole of a substance contains 6.02×10^{23} particles
- This number is known as the **Avogadro constant**.

Therefore, the mass of one carbon atom would be:

$$12 \div 6.02 \times 10^{23}$$

Calculating Moles:

- To calculate the number of moles in a solid, you need to use the following formula:



Now complete the A level exam questions:

1.

What is the number of atoms in 0.0100 mol of NH_3 ?
(The Avogadro constant $L = 6.022 \times 10^{23} \text{mol}^{-1}$)

- A 6.02×10^{25}
- B 1.20×10^{23}
- C 1.81×10^{22}
- D 2.41×10^{22}

(Total 1 mark)

2.

(a) One isotope of sodium has a relative mass of 23.

(i) Define, in terms of the fundamental particles present, the meaning of the term *isotopes*.

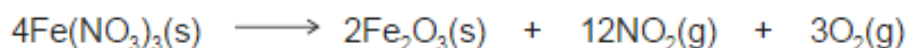
(ii) Explain why isotopes of the same element have the same chemical properties.

(iii) Calculate the mass, in grams, of a single atom of this isotope of sodium.
(The Avogadro constant, L , is $6.023 \times 10^{23} \text{ mol}^{-1}$)

(5)

3.

When heated, iron(III) nitrate ($M_r = 241.8$) is converted into iron(III) oxide, nitrogen dioxide and oxygen.



A 2.16 g sample of iron(III) nitrate was completely converted into the products shown.

(a) (i) Calculate the amount, in moles, of iron(III) nitrate in the 2.16 g sample.
Give your answer to 3 significant figures.

.....
.....

(1)

(ii) Calculate the amount, in moles, of oxygen gas produced in this reaction.

.....
.....

(1)

4.

(a) **Table 1** shows some data about fundamental particles in an atom.

Table 1

Particle	proton	neutron	electron
Mass / g	1.6725×10^{-24}	1.6748×10^{-24}	0.0009×10^{-24}

(i) An atom of hydrogen can be represented as ${}^1\text{H}$

Use data from **Table 1** to calculate the mass of this hydrogen atom.

(1)

(ii) Which **one** of the following is a fundamental particle that would **not** be deflected by an electric field?

A electron

B neutron

C proton

Write the correct letter, **A**, **B** or **C**, in the box.

(1)

(b) A naturally occurring sample of the element boron has a relative atomic mass of 10.8. In this sample, boron exists as two isotopes, ${}^{10}\text{B}$ and ${}^{11}\text{B}$

(i) Calculate the percentage abundance of ${}^{10}\text{B}$ in this naturally occurring sample of boron.

(2)

(ii) State, in terms of fundamental particles, why the isotopes ${}^{10}\text{B}$ and ${}^{11}\text{B}$ have similar chemical reactions.

(1)

5.

(a) Define the term *relative atomic mass*.

An organic fertiliser was analysed using a mass spectrometer. The spectrum showed that the nitrogen in the fertiliser was made up of 95.12% ^{14}N and 4.88% ^{15}N

Calculate the relative atomic mass of the nitrogen found in this organic fertiliser.
Give your answer to two decimal places.

(4)

TASK 3: Bonding Consolidation:

Review your GCSE notes on the different types of bonding. Do some additional research if necessary. Make some summary notes. Include the following types of structures and bonding:

- **Ionic**
- **Covalent: Giant covalent structures and simple molecular structures**
- **Metallic**

Now answer the A level questions below

6.

Which is the correct crystal structure for the substance named?

	Substance	Structure	
A	Iodine	Simple molecular	<input type="checkbox"/>
B	Diamond	Ionic	<input type="checkbox"/>
C	Sodium chloride	Giant covalent	<input type="checkbox"/>
D	Graphite	Metallic	<input type="checkbox"/>

(Total 1 mark)

7.

- (a) (i) Define the term *relative atomic mass* (A_r) of an element.

(2)

- (ii) A sample of the metal silver has the relative atomic mass of 107.9 and exists as two isotopes. In this sample, 54.0% of the silver atoms are one isotope with a relative mass of 107.1

Calculate the relative mass of the other silver isotope.

State why the isotopes of silver have identical chemical properties.

(b) The isotopes of silver, when vaporised, can be separated in a mass spectrometer.

Name the **three** processes that occur in a mass spectrometer before the vaporised isotopes can be detected.

State how each process is achieved.

(6)

(c) State the type of bonding involved in silver.

Draw a diagram to show how the particles are arranged in a silver lattice and show the charges on the particles.

(3)

- (d) Silver reacts with fluorine to form silver fluoride (AgF).

Silver fluoride has a high melting point and has a structure similar to that of sodium chloride.

State the type of bonding involved in silver fluoride.

Draw a diagram to show how the particles are arranged in a silver fluoride lattice and show the charges on the particles.

Explain why the melting point of silver fluoride is high.

(5)

8.

Silicon dioxide (SiO_2) has a crystal structure similar to diamond.

- (a) Give the name of the type of crystal structure shown by silicon dioxide.

(1)

- (b) Suggest why silicon dioxide does **not** conduct electricity when molten.

(1)

- (c) Silicon dioxide reacts with hydrofluoric acid (HF) to produce hexafluorosilicic acid (H_2SiF_6) and one other substance.

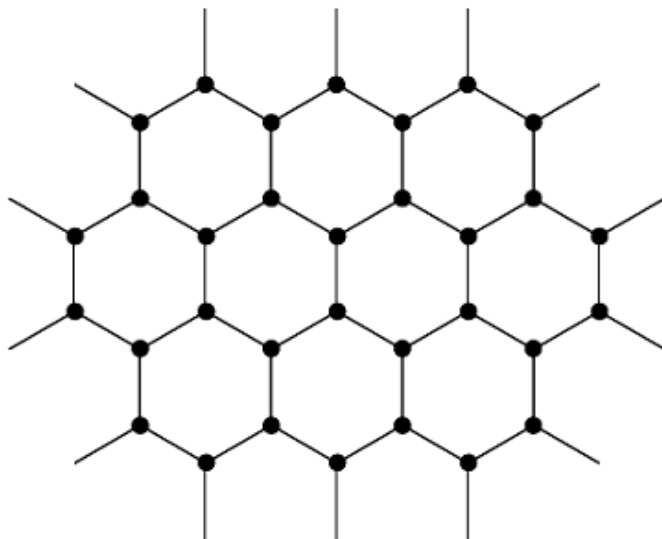
Write an equation for this reaction.

(1)

(Total 3 marks)

9.

- (a) Graphene is a new material made from carbon atoms. It is the thinnest and strongest material known. Graphene has a very high melting point and is an excellent conductor of electricity.
Part of the structure of graphene is illustrated in the diagram.



- (i) Deduce the type of crystal structure shown by graphene.

(1)

- (ii) Suggest why graphene is an excellent conductor of electricity.

(2)

- (iii) Explain, in terms of its structure and bonding, why graphene has a high melting point.

(2)

Titanium is also a strong material that has a high melting point. It has a structure similar to that of magnesium.

- (i) State the type of crystal structure shown by titanium.

(1)

(ii) Explain, in terms of its structure and bonding, why titanium has a high melting point.

(2)

(c) Titanium can be hammered into objects with different shapes that have similar strengths.

(i) Suggest why titanium can be hammered into different shapes.

(1)

(ii) Suggest why these objects with different shapes have similar strengths.

(1)

(d) Magnesium oxide (MgO) has a melting point of 3125 K.
Predict the type of crystal structure in magnesium oxide and suggest why its melting point is high.

Type of crystal structure _____

Explanation _____

(3)

(Total 13 marks)