What is a mass spectrometer?

The *mass spectrometer* is an instrument widely used by chemists, geologists, biologists, physicists and forensic scientists to determine the *relative molecular mass* of atoms and molecules. The spectrometer was invented in 1919 by *Francis W Aston* while working in the world famous Cavendish Laboratories in Cambridge under *JJ Thompson*, the man who discovered the electron.

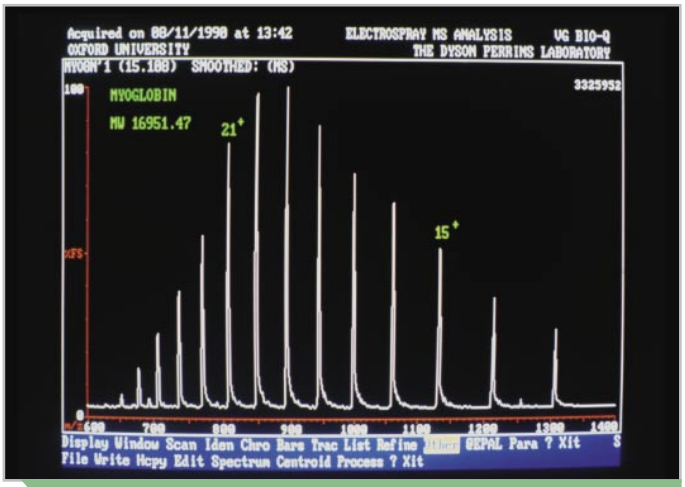


Fig. 1 Mass spectrograph of myoglobin, a muscle tissue protein

What is relative molecular mass?

The relative molecular mass of a substance is defined as the sum of the relative atomic masses of the atoms in a molecule. However, not all atoms of a particular element have the same mass. Such atoms are called *isotopes*.

Frederick Soddy coined the phrase *isotope* while working with lead 206, 207 and 208 which are formed when uranium decays radioactively. He found that atoms of the same element can have the same number of protons but different numbers of neutrons.

Isotopes have the same number of *protons* therefore the same *Atomic Number*. However, they have different numbers of *neutrons* therefore have different *Mass Numbers*. He was awarded the Nobel Prize in 1921 for this work.

Aston initially worked with neon. Using his mass spectrometer, he was eventually able to show that almost all elements have *isotopes*. In fact, he used the mass spectrometer to discover 212 of the 278 naturally occurring isotopes or *nuclides*. He was awarded the Nobel Prize for his work in 1922.

How does the mass spectrometer work?

The spectrometer works on the principle that *ions* can be separated by mass while moving through a magnetic field.

In general, the process of testing a substance follows the sequence:

- Introduction of sample
- vaporisation
- ionisation
- acceleration
- detection
- analysis

We will now look at each stage in turn.

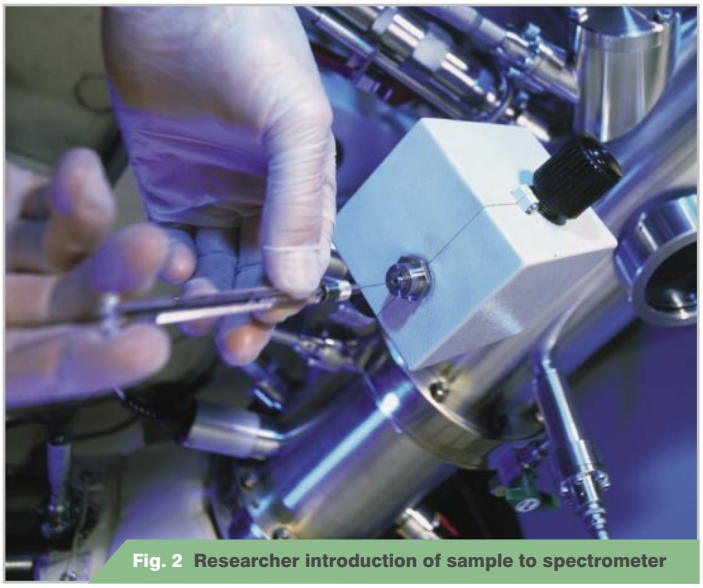


Fig. 2 Researcher introduction of sample to spectrometer

Introduction and vaporisation of a substance

The sample to be tested is introduced to the machine through a *sample inlet*. The sample must then be vaporised. In the case of liquids this is easy as the machine contains a vacuum which lowers the boiling point. However, solids may have to be melted in a special attachment before they are introduced through the sample inlet.

Ionisation of particles

Once inside the particles are *ionised*. They are bombarded by high energy electrons which are boiled off a hot negatively charged wire, often referred to as the *electron gun*. The negative charge on the wire repels these electrons [like charges repel], while the *anode* attracts them [unlike charges attract]. Thus, the electrons move at great speed. These high energy electrons strike the molecules and knock other electrons off them and, in doing so, turn the molecules into positive ions.

Acceleration of the ions in a charged field

These positive ions are attracted by a series of negatively charged plates in the *accelerator*. Some of the ions pass through a tiny hole in the centre of these plates. This forms a narrow beam of positive ions passing into the *analyser unit*. There are no air molecules in the machine to hinder the movement of the ions, so they move at great speed into the analyser unit.

The particles are separated by mass, using a varying magnetic field

The ions are then subjected to a *magnetic field* in the analyser. This magnetic field deflects the ions. The degree of deflection depends on the mass of the particles and the strength of the magnetic field. The stronger the magnetic field, the greater the deflection. Also the lighter a particle, the greater its deflection. By adjusting the magnetic field, ions of a particular mass can be made to fall on the *detector*, where they produce a small electric current. By gradually increasing the magnetic field ions of greater mass can be brought in turn to focus on the detector.

This is followed by amplification of the signal produced

The detector is very sensitive, and the signal is amplified electronically and displayed on a computer monitor. At the same time, it is printed as a *spectrograph*. This spectrograph gives the mass of the ions along the horizontal axis and their *relative abundance* on the vertical axis.

Interpretation of data or spectrograph

In the spectrograph the percentage of each ion can be determined by calculating its fraction of the total abundance. This is called the *relative abundance* of an isotope. This is done by comparing the length of the line with the sum total length of all the lines.

What is the mass spectrometer used for?

Until about 1970, the mass spectrometer was used to identify and analyse the abundance of isotopes. Since then it has been modified to determine the masses of unknown organic compounds and help determine their structures. The ionisation process breaks up the compound into smaller fractions each of which forms a trace. All of these traces form a complex mass spectrum characteristic of the initial compound. Research establishments have data banks of the mass spectrographs of compounds and scientists can draw on them to readily identify compounds, for example to identify gases produced by waste dumps and trace organic pollutants in water. The spectrometer is also used in drug testing.

A worked example

An element is found to have two isotopes with the following abundances 55% ^{63}X and 45% ^{64}X. We can identify it by calculating the *relative atomic (A_R) mass*, as follows.

$$\frac{(55 \times 63) + (45 \times 64)}{100} = \frac{3465 + 2880}{100} = \frac{6345}{100} = 63.45\text{g/mol}$$

This indicates that the element is Copper (Cu).

HEA
Higher Education Authority
An tÚdarás um Ard-Oideachas

The Higher Education Authority and the PRTLI

Ireland's future prosperity requires that a knowledge-based society be created. The goal is to develop a society where social development, quality of life and personal growth are enhanced through innovation in a thriving economy.

The **HEA (Higher Education Authority)** is playing a key role in this. The HEA advises the government and it provides much funding in higher education through the PRTLI, an investment vehicle intended to transform Irish research. The **PRTLI (Programme for Research in Third Level Institutions)** allows third-level institutions to build infrastructure and provide a career-path for talented researchers. Its funds, combined with those from other funding bodies, are creating a first class research ecosystem in Ireland. You can find out more about the HEA at **www.hea.ie**.

The scale of the investment is significant. To date, PRTLI funding has exceeded €600 million in some years. The PRTLI invests in infrastructure (buildings and equipment) and the researchers who use it. Thirty-three research centres will be provided when the programme is complete.

One such centre is the **Analytical and Biological Chemistry Research Facility (ABCRF) at University College Cork.** The researchers here carry out complex analytical work on important biological molecules, from the smallest to the largest macromolecule, which might contain millions of atoms. In doing so, these researchers use the most advanced and sophisticated instruments and equipment - spectroscopy, holography, crystallography and mass spectrometry.

You can out more about the ABCRF and these research projects at **http://abcrf.ucc.ie** and at **www.sciencetechnologyaction.com**

Syllabus Reference

Leaving Certificate Chemistry:

Section 1.2 – Atomic Structure
Section 7.5 – Instrumentation

Learning Objectives

On completing this lesson the student should be able to:

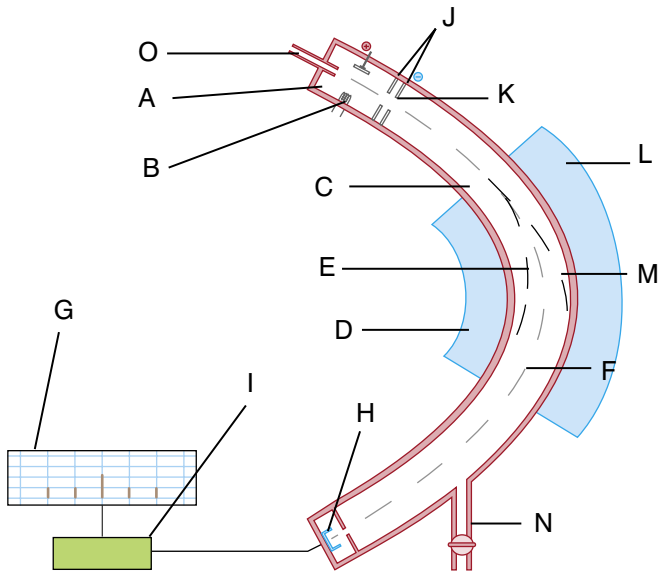
- Describe the Mass Spectrometer
- Identify the inventor of the instrument
- Define the term isotope
- Name the components of the instrument and their function
- Describe the process of testing a substance
- Nominate some practical uses for the instrument

General Learning Points

- The mass spectrometer is used to determine the relative atomic mass and relative molecular mass of chemical substances.
- It was invented by F. W. Aston in 1913.
- Aston continued to refine the spectroscope and eventually identified 212 of the currently known isotopes.
- Isotopes were discovered and named by Frederick Soddy.
- Because an element could have many isotopes, each with a different mass, the tabulated atomic masses of elements are averages of these isotopes.
- It is very difficult to measure atomic weights with absolute precision. Following international agreement between chemists and physicists, relative atomic masses are now based on the isotope of carbon which has mass number 12. This isotope is known as carbon 12 or ^{12}C.
- The sample must be vaporised so that particles can more easily be bombarded with electrons.
- The quantity of an isotope in a sample is known as its relative abundance.
- Chemical laboratories often hold databases of thousands of spectra for comparative purposes.

Activities

1. Review the stages through which a test substance passes in the Mass Spectrometer.
2. Label the components shown in this diagram of the Mass Spectrometer.



Examination Questions

2002 Higher Level

Mass spectrometry and gas chromatography are widely used instrumental techniques in chemistry.

(a) Give one application of each of these techniques. (8)
(b) What are the main principles on which each of these techniques are based? (18)
(c) What are the fundamental processes that occur in a mass spectrometer? (15)
(d) HPLC is another chromatographic technique.
What do the letters HPLC stand for? State one application for this technique. (9)

For further examples of past paper exam questions check out www.sciencetechnologyaction.com

True or False

Indicate whether the following are true (T) or false (F) by drawing a circle around T or F.

(a) The Mass Spectrometer was invented by Albert Einstein.	T	F
(b) Isotopes of the same element have the same relative atomic mass.	T	F
(c) Isotopes were discovered by Frederick Soddy.	T	F
(d) When high energy electrons hit a sample molecule they knock protons off the molecule.	T	F
(e) In the magnetic field heavy particles are deflected more than light ones.	T	F
(f) Heavy particles are separated because they fall under the influence of gravity.	T	F
(g) A spectrograph shows mass on the horizontal axis and abundance on the vertical axis.	T	F
(h) A substance is vaporised before introduction to the mass spectrometer.	T	F
(i) Aston did his initial work on neon.	T	F
(j) All elements have isotopes.	T	F

Check your answers to these questions on www.sciencetechnologyaction.com

Did You Know?

- Aston's ingenious use of electromagnetic focusing enabled him to separate the very small differences in mass of isotopes.
- The detector in Aston's first spectrometer was a photographic plate.
- Francis Aston was an athletic person. He excelled at skiing, tennis, rock climbing and swimming. He also played the piano, violin and cello.
- Sir J.J.Thomson invited him to work as his assistant at the Cavendish Laboratory, Cambridge, on studies of positive rays.
- It is said that Margaret Todd suggested the word isotope to Frederick Soddy.
- The word isotope comes from the Greek - *isos* meaning *equal* and *topos* meaning *place*. The isotopes have different atomic massess, but occupy the same place on the Periodic Table.
- There are 114 known elements but over 3000 known isotopes.

Biographical Notes

Francis William Aston

was born in England in 1877. His interest in science was aroused while still at school. At one stage he worked a chemist in the laboratory of a brewery. Here, he showed his great aptitude for mechanical invention and designed many pumps for evacuating containers. His great invention is the *mass spectrometer*. He discovered no less than 212 of the naturally occurring isotopes. He won the Nobel Prize for Chemistry for 1922. He died in 1945.

Frederick Soddy

was also born in England in 1877. As a young man he worked with the famous *Ernest Rutherford* at McGill University, Montreal on problems of radioactivity. He also worked with *Sir William Ramsay* at University College, London where he studied radioactivity. His great accomplishment is the concept of *isotopes*. He won the Nobel Prize for Chemistry in 1921. He died in 1956.

You can find out more about these and other great scientists at www.sciencetechnologyaction.com

Revise the Terms

Can you recall the meaning of these terms? Revising terminology is a powerful aid for recall and retention

Mass spectrometer; relative molecular mass; relative atomic mass; isotopes; protons; neutrons; atomic number; mass numbers; nuclides; ions; sample inlet; ionised; electron gun; anode; accelerator; analyser unit; magnetic field; detector; spectrograph; relative abundance.

Check the Glossary of Terms for this lesson at www.sciencetechnologyaction.com