

A proposal to introduce a topic of contemporary physics into high-school teaching

Wilma M S Santos, Adir M Luiz and Carlos R de Carvalho

Instituto de Física, Universidade Federal do Rio de Janeiro, Caixa Postal 68528, 21941-972, Rio de Janeiro, RJ, Brazil

E-mail: wilma@ifufrj.br

Abstract

This article presents an approach to integrate contemporary physics into high-school teaching. We present a simple way to understand mass spectroscopy using basic physics concepts, so that high-school students may have contact with recent topics of modern research. The main features of a time-of-flight (TOF) mass spectrometer using secondary school physics concepts are discussed. The use of home-made apparatus is described. Some results obtained with CsI samples showing the dependence between mass and TOF are presented.

Introduction

For a long time there has been worldwide concern about introducing the study of modern science, in particular contemporary physics, into secondary schools [1–4]. For instance, the introduction of modern science in Japan dates back to the second half of the nineteenth century. After the Second World War, Japan's educational system underwent a reform in which one of the rules was based on the spread of scientific culture and the improvement of scientific standards for all levels of the educational system [5]. One also finds such concerns in the speech of USA's President Clinton in which he established a direct connection between the learning of mathematics and science and success in obtaining better jobs [6]. The search for the highest educational standards leads sometimes to controversies [7], but this reflects the importance that is given to this subject nowadays. In fact the dissemination of scientific knowledge can be found in international policy. The evidence of this

is the existence of organizations such as UNESCO and its initiatives on this subject [8].

This article intends to bring to high-school classes problems of current scientific research. For this purpose we have chosen the problem of mass spectrometry, also known as mass spectroscopy (MS); it is a subject of practical as well as academic interest and uses simple physics concepts in the analyses of the experimental results. These are important aspects when one chooses a subject to discuss with secondary students; one should be able to answer a common question: 'what's that stuff for?'. A subject that has both practical and academic applications is interesting because it covers all ranges of curiosity of young students.

In the following sections, we first discuss briefly the history and the technical features of MS. Afterwards, we discuss the use of a home-made camera that has been used in our experimental set-up as a time-of-flight (TOF) mass spectrometer. In this type of spectrometer, the mass of the

ions is obtained by measuring the TOF of the ions when they are accelerated by electric fields. Therefore, by making use of basic kinetic and electric concepts we shall present the analysis which gives the mass of the ions as a function of the time that they spend going from the sample to the detector. Next, we show some experimental results obtained with CsI samples. Finally, we present some conclusions.

Mass spectroscopy: history and general features

Just as fingerprints are used to identify people, spectrometry is used to identify substances. There are many types of spectrometric techniques to identify molecules. For neutral molecules, the best techniques are based on the analysis of spectra obtained using electromagnetic waves emitted by the molecules. Optical spectra and infrared spectra are examples of the latter techniques. However, to identify charged molecules or atoms, mass spectrometry is commonly used.

Mass spectroscopy is an analytical tool used to determine the basic compounds of a sample. More specifically, it is usually used for elucidating the chemical structures of the substances. In order to measure the individual components of the molecules, a mass spectrometer converts them to ions so that they can be moved about by external electric and magnetic fields. Thus, a mass spectrometer is composed of an ion source, an analyser that separates the molecular ions according to their mass-to-charge ratio, an ion detector and a data acquisition system.

The ions are generated in the ion source by inducing either the loss or the gain of a charge. Once the ions are formed in the gas phase they can be electrostatically directed into a mass analyser, separated according to mass and finally detected. The result of ionization, ion separation and detection is a mass spectrum that can provide molecular weights or even structural information.

Today's mass spectroscopy is based on the famous work performed by J J Thomson of the Cavendish Laboratory of the University of Cambridge, UK. Thomson's research, which led to the discovery of the electron in 1897, also led to the first mass spectrometer while he was measuring the effects of electric and magnetic fields on ions generated by residual gases in

cathode ray tubes. Thomson established the 'mass-to-charge' ratio for the electron analysing the deflections of the cathode rays due to magnetic and electric fields and received the 1906 Nobel Prize in Physics for this discovery [9].

Mass spectrometers have become very important tools for a wide range of applications in the analysis of inorganic, organic and biological substances. Examples include dating of geological samples, drug discovery, processes used in the petroleum, chemical and pharmaceutical industries, surface analysis of materials, analysis of macromolecules, research in DNA sequencing and analysis of viruses.

In modern spectrometers, the most important techniques used for the ionization of the samples to be analysed are: electron ionization (EI), spontaneous desorption (SD), electrospray ionization (ESI) and matrix-assisted laser desorption-ionization (MALDI).

EI, formerly known as electron impact, is an ionization method in which energetic electrons interact with atoms or molecules to produce ions. This method is particularly used for organic molecules due to the efficiency of ionization and the production of fragment ions, for the typical energy range of electrons beams found in scientific laboratories [10]. The EI technique is straightforward. The sample must be delivered as a gas which is usually accomplished by heating the sample to vaporize it from the probe. Once in the gas phase, the compound passes into an electron ionization region where it interacts with a beam of electrons of nearly homogeneous energy (70 eV)¹, typically causing electron ejection and some degree of fragmentation.

In spontaneous desorption (SD) the ionization is performed using electrostatic fields without the use of incident beams of electrons [11]. This technique was developed initially in 1985 [12].

Electrospray ionization (ESI) generates ions directly from solution (usually an aqueous or aqueous-organic solvent system) by creating a fine spray of highly charged droplets in the presence of a strong electric field (typically 3.5 kV) [13].

In 2002, the Nobel Prize in Chemistry was awarded to John Bennett Fenn [14] for the

¹ *Electronvolt* (eV) is a convenient unit for electronic energies and is defined as the energy acquired by an electron accelerated through a potential difference of 1 volt (V). Since $e = 1.6 \times 10^{-19}$ C and 1 Joule (J) = 1 V \times 1 C, then 1 eV = $(1.6 \times 10^{-19} \text{ C}) \times 1 \text{ V} = 1.6 \times 10^{-19} \text{ J}$.

development of electrospray ionization (ESI) and Koichi Tanaka [15] for the development of soft laser desorption (SLD) presently known as matrix-assisted laser desorption-ionization (MALDI).

Matrix-assisted laser desorption-ionization mass spectrometry (MALDI-MS) was first introduced in 1988 by Tanaka [15] and independently by Karas and Hillenkamp [16] and it has become a widespread analytical tool for peptides, proteins and most other biomolecules.

Concerning the MS analyser one also finds different kinds of mass analysers to separate the ions, the better known of which include *magnetic sector*, *time of flight* (TOF), *quadrupoles* and both *Fourier transform* and *quadrupole ion traps* [10]. In our experiments we have used a TOF analyser. Unlike the others, the TOF analyser is very simple to describe using elementary physics concepts and thus is particularly useful for secondary school students, considering their level of knowledge.

Finally, the detector monitors the ion current, amplifies it and the signal is then transmitted to the data acquisition system, where it is recorded in the form of mass spectra (counting \times compound mass), which gives the *relative abundance* of the various components versus the *mass* of each component in the sample.

Another type of MS is *accelerator mass spectrometry* (AMS). AMS differs from the other forms of MS previously described in that it employs an accelerator to accelerate ions to high kinetic energies (above MeV) before mass analysis. AMS is most often employed to determine the concentration of ^{14}C , a fundamental technique used by archaeologists for radiocarbon dating [17].

In this article, we describe a particular TOF MS with a home-made MALDI camera in order to study MS.

Experimental set-up

In our experimental set-up a pulsed laser was used to bombard a composite solid. The laser pulses are in the ultraviolet range (wavelength = 337.1 nm), with time width between 3 and 4 ns, and a mean energy per pulse equal to 120 μJ . The interaction of the laser pulse with the sample produces ions in the gas phase (ionic desorption). The ion cloud contains a mixture of ionic and neutral fragments that are separated by the spectrometer. An electric

field applied between the sample at high voltage (~ 10 kV) and a grounded grid accelerates the ionized molecules towards the detector.

The desorbed ions have an initial kinetic energy distribution with a mean value of the order of 10 eV. These ions are accelerated and collide with a microchannel plate detector (MCP) giving signals to be used in the TOF measurements. In figure 1 we show a sketch of our experimental set-up and figure 2 shows a detail of this set-up.

Time-of-flight analysis

TOF analysis is generally based on accelerating a set of ions to a detector. In this section we show the basic equations necessary for the calculation of the TOF and how to obtain the mass of an ion using the appropriate equations or using the experimental values of the TOF.

Consider a fragment produced by laser desorption-ionization with a kinetic energy $E = \frac{1}{2}mv^2$. Its initial velocity is then given by

$$v = \sqrt{\frac{2E}{m}} \quad (1)$$

where m is the fragment's mass. As mentioned in the previous section, the corresponding energy is of the order of 10 eV which is appreciably greater than the thermal energy at room temperature $k_{\text{B}}T \sim 1/40$ eV, where k_{B} is the Boltzmann constant. Once the subject is focused for high-school students, the teacher should mention that the ions are produced by the laser with energy considerably greater than the thermal energy, otherwise the ions would not be desorbed.

The ion cloud contains charged fragments (ions). All these particles are separated by the spectrometer through an applied electric field, which is accomplished by a difference of electric potential between the sample plate and a grid in front of it (see figure 1).

Let us now consider an ion moving along the region of length L_1 between the sample and the grid under the influence of the electric field. If this ion has a net charge Q and is accelerated due to the electric field, which we suppose to be uniform for simplicity, the kinetic energy increase in a section of length L_1 of the spectrometer is given by

$$\frac{1}{2}(mu^2 - mv^2) = QV_0 \quad (2)$$

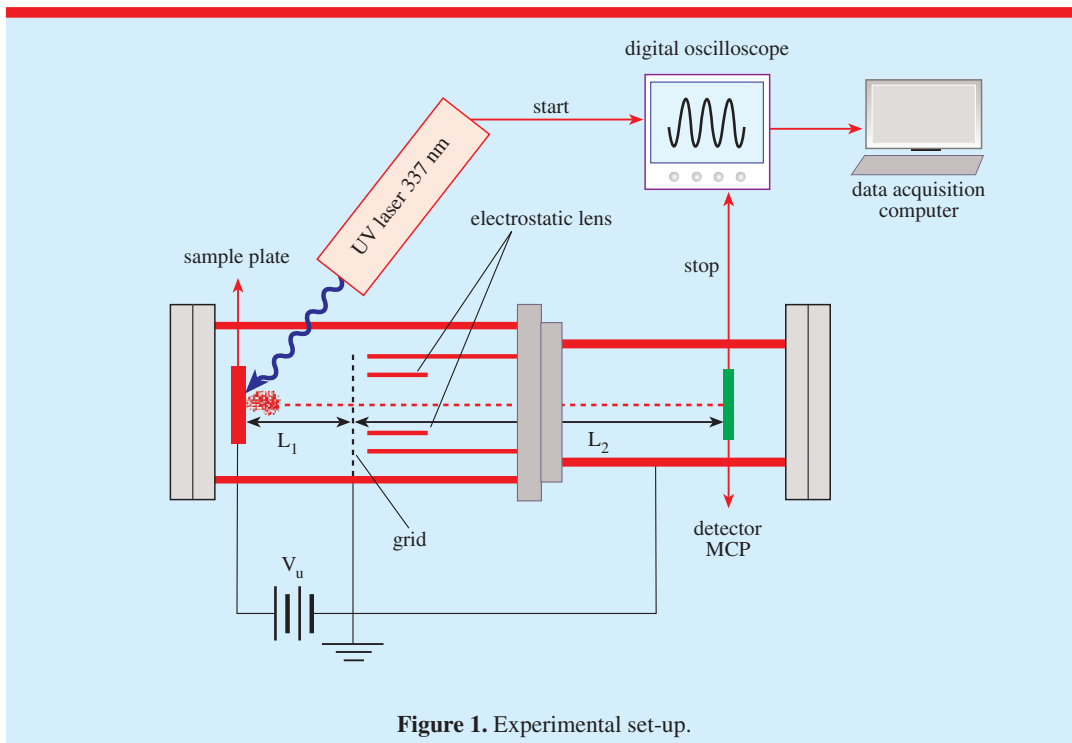


Figure 1. Experimental set-up.



Figure 2. Detail showing the home-made MALDI camera and the laser.

where V_0 is the electric potential difference across the length L_1 , u is the final velocity of the particle and v is the initial velocity obtained by equation (1). In figure 1 the electric potential V_0 is approximately equal to 10 kV. As we have mentioned, the desorbed ions have kinetic energies approximately equal to 10 eV. Thus, considering equation (1) we may neglect the initial velocity v in equation (2).

For a constant acceleration a across the length L_1 , the corresponding TOF t_1 is given by

$$t_1 = \sqrt{\frac{2L_1}{a}}. \quad (3)$$

In the region considered there is a constant electric field, whose modulus is V_0/L_1 . Therefore the electric force is given by

$$F = Q \frac{V_0}{L_1}. \quad (4)$$

On the other hand, by Newton's second law, we know that

$$F = ma. \quad (5)$$

By equations (4) and (5), we obtain

$$a = \frac{QV_0}{mL_1}. \quad (6)$$

From the equations (3) and (6) we obtain for the TOF of the particle in the first section the following expression:

$$t_1 = L_1 \sqrt{\frac{2m}{QV_0}}. \quad (7)$$

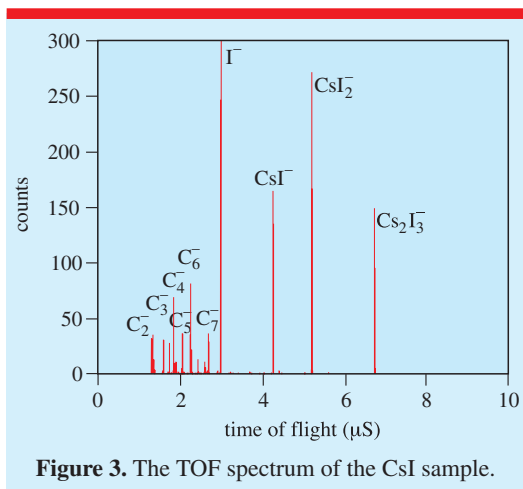


Figure 3. The TOF spectrum of the CsI sample.

Along the length L_2 , between the grid and the detector, the electric field is equal to zero and the ion's motion is uniform, i.e. the velocity is constant. Thus, in this second part, the TOF t_2 is given by

$$t_2 = \frac{L_2}{u} \quad (8)$$

where u is the final velocity of the accelerated motion in the first part. Because we have neglected the initial velocity v of the desorbed ion, the final velocity u is given by:

$$u = at_1. \quad (9)$$

According to equations (6)–(8), one finds

$$u = \sqrt{\frac{2QV_0}{m}}. \quad (10)$$

Thus, substituting equation (10) in (8) one finds

$$t_2 = L_2 \sqrt{\frac{m}{2QV_0}}. \quad (11)$$

Finally, the resulting TOF t along the whole spectrometer is the sum $t_1 + t_2$:

$$t = \left[\frac{1}{\sqrt{QV_0}} \left(L_1 \sqrt{2} + \frac{L_2}{\sqrt{2}} \right) \right] \sqrt{m} = A \sqrt{m} \quad (12)$$

where the constant A is the expression between the brackets.

Equation (12) is frequently used for TOF analysis. The resolution of a mass spectrometer can be defined simply as its ability to separate two ions of different mass. Equation (12) shows that in

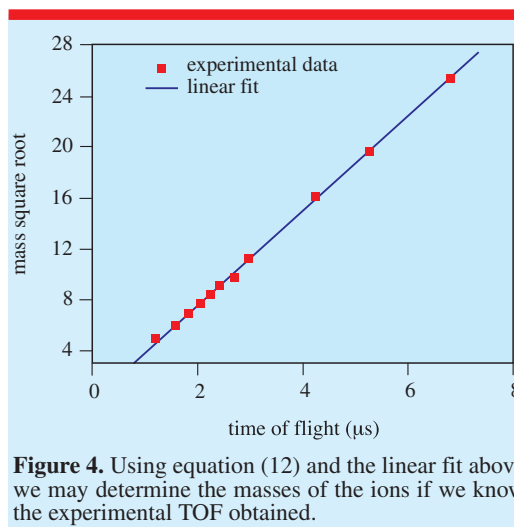


Figure 4. Using equation (12) and the linear fit above we may determine the masses of the ions if we know the experimental TOF obtained.

a linear MALDI-TOF instrument the total TOF t depends on the lengths L_1 and L_2 of the sections considered. Equation (12) also shows that t is a linear function of the square root of the mass.

It is important to mention that, for simplicity, we have used for V_0 a positive value (the modulus of the electric potential difference) in all the previous equations. However, in the experiments performed, the sample plate has been biased by a negative potential difference, that is, only negative ions are accelerated in the initial section of the apparatus. Thus, in the experimental results presented in the next section, only negative ions have been detected in the MCP detector indicated in figure 1.

Results

In figure 3 we show the experimental TOF spectrum obtained with a CsI sample. This TOF spectrum shows the negative ions obtained from the CsI sample. The linear fit obtained for this spectrum is indicated in figure 4, corroborating the linear relationship between the mass square root and the TOF, as equation (12) shows. Some ions of carbon are also indicated in figure 3. These ions were produced because the camera has been contaminated by carbon atoms remaining in the camera from a previous experiment performed with carbon.

Conclusions

This work suggests that the proposal of teaching a topic of contemporary physics research, such

as mass spectroscopy, is valuable for students as well as for teachers. The equations used in the mass calculations of the ions are very simple. The study of mass spectroscopy has both practical and academic interest because it covers basic classical and modern physics concepts. Students that have visited our laboratory found the project fun, creative and instructive. We hope that our proposal will be helpful for physics teachers when they explain topics of contemporary physics.

Received 31 March 2009, in final form 29 May 2009
doi:10.1088/0031-9120/44/5/011

References

- [1] Kapon S, Ganiel U and Eylon B 2009 Scientific argumentation in public physics lectures: bringing contemporary physics into high-school teaching *Phys. Educ.* **44** 33–8
- [2] Peralta L, Farinha A and Pinto A 2008 X-ray detection visits the classroom *Phys. Educ.* **43** 350–2
- [3] Planinšič G and Kovač J 2008 Nano goes to school: a teaching model of the atomic force microscope *Phys. Educ.* **43** 37–45
- [4] Dhési S and Smith D 2007 Interview: Diamond synchrotron prepares to light up x-ray optics in the UK *Phys. Educ.* **42** 106–9
- [5] Japan's Modern Educational System (Ministry of Education, Culture, Sports, Science and Technology—Japan) 2009 See chapter VI and chapter VIII in www.mext.go.jp/b_menu/hakusho/html/hpbz198103/index.html
- [6] Clinton B 1997 Speech to the NAACP National Convention on 17 July <http://clinton4.nara.gov/WH/New/html/19970908-7174.html>
- [7] Lipsett A 2008 Science and maths assaulted by educational reforms, say scientists *Guardian* 5 September www.guardian.co.uk/education/2008/sep/05/1419education.schools
- [8] Quere Y and Jasmin D 2005 When learning science becomes child's play *A World Sci.* **3** 2–8
- [9] Weinberg S 1993 *The Discovery of Subatomic Particles* (London: Penguin Books)
- [10] Ashcroft A E 1997 *Ionization Methods in Organic Mass Spectrometry* (Cambridge: RSC Publishing)
- [11] Salehpour M and Hunt J E 1988 Spontaneous desorption mass spectrometry: applications and mechanisms *Int. J. Mass Spectrom. Ion Process.* **85** 99
- [12] Della-Negra S, Le Beyec Y and Haconsson P 1985 Spontaneous desorption time-of-flight mass spectrometry (SDMS): time correlated emission of electrons and negative ions in a constant electric field *Nucl. Instrum. Methods B* **9** 103
- [13] Cole R (ed) 1997 *Electrospray Ionization Mass Spectrometry: Fundamentals, Instrumentation, and Applications* (New York: Wiley)
- [14] Fenn J B, Mann M, Meng C K, Wong S F and Whitehouse C M 1990 Electrospray ionization—principles and practice *Mass Spectrom. Rev.* **9** 37
- [15] Tanaka K, Waki H, Ido Y, Akita S, Yoshida Y and Yoshida T 1988 Protein and polymer analyses up to m/z 100 000 by laser desorption time-of-flight mass spectrometry *Rapid Commun. Mass Spectrom.* **2** 151
- [16] Karas M and Hillenkamp F 1988 Laser desorption ionization of proteins with molecular masses exceeding 10 000 daltons *Anal. Chem.* **60** 2299
- [17] Budzikiewicz H and Grigsby R D 2006 Mass spectrometry and isotopes: a century of research and discussion *Mass Spectrom. Rev.* **25** 146

Wilma Machado Soares Santos has been an Associate Professor at the Physics Institute of the Federal University of Rio de Janeiro (UFRJ), Brazil for 31 years. She researches in atomic and molecular physics, and has also been developing research in physics education.

Adir M Luiz is an Associate Professor at the Physics Institute of the Federal University of Rio de Janeiro (UFRJ), Brazil. He has taught university physics for 40 years. He researches in superconductivity and mass spectrometry.

Carlos Renato de Carvalho has been an Associate Professor at the Physics Institute of the Federal University of Rio de Janeiro (UFRJ), Brazil for 16 years. His main interests are in quantum optics and quantum information.