

Mass spectrometry in modern physical research methods

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ABSTRACT

History of development and improvement of tandem mass spectrometry, possibilities of its application at the contemporary stage in various fields of medicine and biotechnology including production of novel medicinal preparations, identification of biologically active substances, pathogenic microorganisms and causative agents of especially dangerous infections is given.

Keywords:

Mass spectrometry, pharmacology; identification of biologically active substances, pathogenic microorganisms and causative agents of especially dangerous infections

Introduction

In 1952, the English scientist A. J. Martin and his collaborator A. James, while analyzing fatty acids, made two very important observations. First, they discovered that chromatography can separate not only dissolved liquid substances, but also gases and vapors. Secondly, they showed that separation can be carried out without only through repeated repetition of the adsorption-desorption cycle, but also through alternating absorption and desorption. The words adsorption and absorption differ from each other by one letter, but are used they refer to completely different processes.

Adsorption is concentration of a substance at the interface between phases (solid-gaseous, solid-vapor, solid-liquid). During absorption, solutions, gases or vapors also come into contact with the liquid phase, but the molecules of these substances do not linger on the interface, but are absorbed, that is, dissolved, in the volume of the liquid and solid[1-16].

Phenomena associated with the absorption of gases in liquids underlie gas-liquid chromatography, the most common separation method currently used. When there is a gas above a liquid solution, a dynamic relationship is established between the gas molecules that

dissolve in the liquid and those that remain in the gas phase.

equilibrium. If above the liquid there is not an individual gas, but a mixture of gases and this the mixture begins to move, then the individual components of the gas mixture, having different solubilities in this liquid, move at different speeds.

In the end, the gas mixture will separate into its component parts. As can be seen, the principle of separation of liquid mixtures proposed by Tsvet can also be used for the analysis of gas mixtures.

The application and analytical qualities of mass spectrometry are mainly determined by the possibility of combining it with other methods such as gas chromatography, high performance liquid chromatography, capillary electrophoresis and pyrolysis. One of the first places in organic analysis is occupied by chromatography-mass spectrometry, which provides high selectivity of detection due to the direct correlation of the obtained data with the structure of organic molecules, as well as the possibility of detecting unknown compounds in complex mixtures. It is of particular importance for the control of environmental pollution, biological fluids, food and technical materials, components.

The connection of a gas chromatograph using large-diameter capillary columns and a mass spectrometer is carried out through a special interface that serves to reduce the gas flow entering the mass spectrometer by draining excess carrier gas and enriching the gas flow with analytes. In the case of ordinary (0.25 and 0.32 mm) and small (less than 0.2 mm) diameter capillary columns, the end of the column is inserted directly into the ion source of the mass spectrometer, and the entire gas flow enters the ion source. The liquid chromatograph and mass spectrometer are also connected using an interface that removes most of the liquid phase from the sample

before it enters the mass spectrometer. Various interfaces have been proposed for mass spectrometry integration: moving conveyor, thermal jet, electric jet, with atmospheric pressure ionization, with glow.

Method and results

Currently, atmospheric pressure electro-sputter and ionizing devices are mainly used for removing the liquid phase and ionizing the molecules of the analyzed substances.

Chromatography-mass spectrometry data are analyzed in two ways. According to the first method, the mass spectra recorded at different points of the mass chromatogram are analyzed by comparison with the mass spectra of the standards collected in the database (library search) or the components of the molecule are determined using spectro-structural correlations. According to the second method, mass chromatograms are recorded and analyzed for total ion flux, individual ions or groups of ions. Such ion mass chromatograms allow the determination and confirmation of the structure of the components of a mixture and the selective separation of homologous series. Additional discriminating factors are used to increase selectivity. This can be the production of derivatives or the use of selective ionization methods that allow the identification of certain functional groups. Photoionization selectively affects molecules with an ionization potential above a certain threshold (the greatest selectivity is achieved in the case of resonant photoionization), with negative chemical ionization, the probability of formation of ions of compounds with high electron affinity increases. Additional methods of selecting the formed ions are also used, for example, high-resolution mass spectrometry, when only ions with a certain elemental composition are recorded, or to record the ions formed as a result of specified decay processes

of selected molecular or decay ions. tandem

mass spectrometry that provides (fig-1).

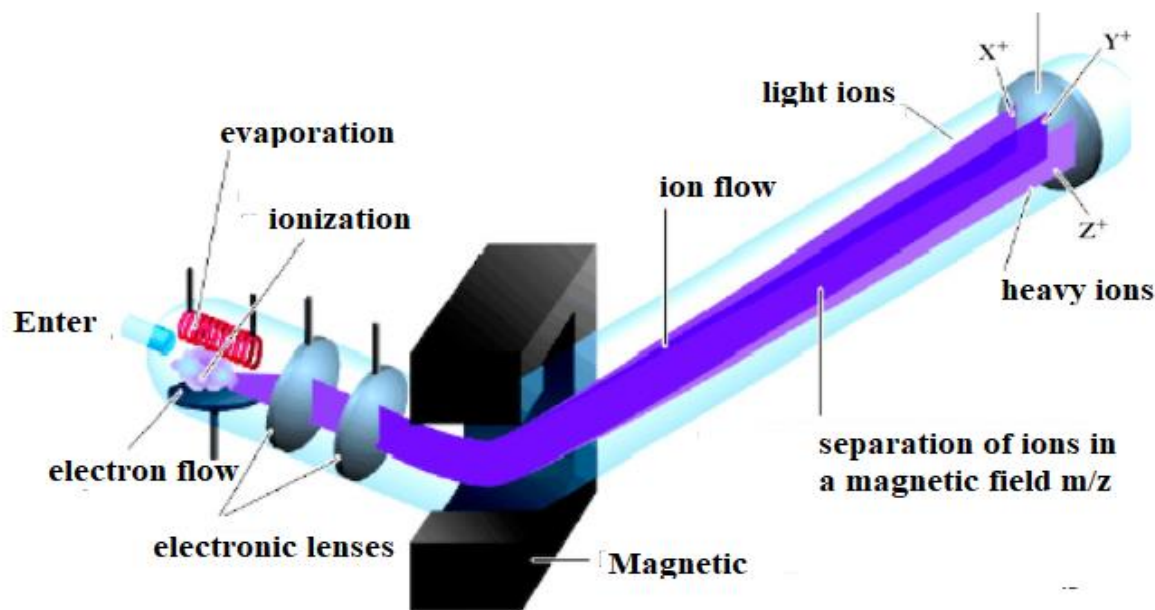


Fig-1
Excremental part

Large assistance in identification is provided by the bank of mass spectral data, which the customer receives along with the device. As mass spectrometry analyzes progress new results are continuously entered into the computer's memory, replenishing the data bank.

If it is necessary to use the bank, the analyst sends a request to the computer, and the computer itself finds in memory the spectrum that best matches the one recorded in the computer. The current spectrum. Both spectra appear on the screen, and now all that remains is to compare the two spectral patterns. Comparison of spectra, that is, a kind of fingerprint identification, is much easier for identifying unknown substances than reconstructing molecules from individual fragments. The only necessary condition for such identification is the presence in the data bank of the spectrum of the very substance that was received for analysis.

Conclusion

Chromatography-mass spectrometry has found wide application in various fields of chemistry, medicine, pharmaceutical production, environmental monitoring and technological control in industry.

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