Chromatography-Mass Spectrometry in Modern Physical Research Methods

[1]Khaydarov Gayrat Shoyimovich	[1]Uzbekistan-Finland Pedagogical Institute, Faculty of Natural and Physical Culture, Department of Natural Sciences
[1]Kholmirzaev Mekhroj Murodillayevich	[1]Uzbekistan-Finland Pedagogical Institute, Faculty of Natural and Physical Culture, Department of Natural Sciences
[1]Tilyabov Makhsudjon Umurzkhovich	[1]Uzbekistan-Finland Pedagogical Institute, Faculty of Natural and Physical Culture, Department of Natural Sciences
[2]Abdusoliev Shakzod Sharafiddin o'g'li	[2]Student Uzbekistan-Finland Pedagogical Institute, Faculty of Natural and Physical Culture, Department of Natural Sciences
[3]Saitkulov Foziljon Ergashevich	Tashkent State Agrarian University

ABSTRACT

Chromatography-mass spectrometry data is analyzed in two ways. According to the first method, the mass spectra recorded at various points of the mass chromatogram are analyzed by comparison with the mass spectra of the standards collected in the database

Keywords: Chromatography, mass spectrometry, first method, various points, mass spectra of the standards collected, high performance liquid chromatography, capillary electrophoresis and pyrolysis

Introduction

The applicability and analytical qualities of mass spectrometry are largely determined by the possibility of its combination with other methods, such as gas chromatography, High performance liquid chromatography, capillary electrophoresis and pyrolysis [1]. One of the first places in organic analysis is occupied by chromatography-mass spectrometry, which, due to the direct connection of the data obtained with the structure of organic molecules, provides high selectivity of determination, as well as the possibility of identifying unknown compounds in complex mixtures. This is of particular importance for the control of environmental pollution, components of biological fluids, food and technical materials [2].

Methods And Results

The connection of a gas chromatograph using large-diameter nozzle and capillary columns and a mass spectrometer is carried out through a special interface that serves to reduce the flow of gas entering the mass spectrometer by dumping excess carrier gas and enriching the gas stream with analyzed substances. In the case of capillary columns of ordinary (0.25 and 0.32 mm) and small (less than 0.2 mm) diameter, 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 [3-16]. 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. Many different types of interfaces have been proposed for combining HPLC and mass

spectrometry: moving conveyor, thermal jet, electric jet, with ionization at atmospheric pressure, with glow discharge, etc. Currently, devices with electro-sputtering and ionization at atmospheric pressure are mainly used, which perform the functions of removing the liquid phase and ionization of the molecules of the analyzed substances [4].

The Experimental Part

Chromatography-mass spectrometry data is analyzed in two ways. According to the first method, the mass spectra recorded at various points of the mass chromatogram are analyzed by comparison with the mass spectra of the standards collected in the database (library search), or the structural fragments of the molecule are determined using spectro-structural correlations. According to the second method, mass chromatograms are recorded and analyzed for the total ion current, for individual ions or groups of ions. Such ionic mass chromatograms make it possible to detect and confirm the structure of the components of the mixture and selectively isolate homologous series. Additional discriminating factors are used to increase selectivity. This may be the production of derivatives that allow the identification of certain functional groups, or the use of selective ionization methods. 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 selection of formed ions are also used, such as high-resolution mass spectrometry, when only ions with a certain elemental composition are recorded, or tandem mass spectrometry, which provides registration of ions formed as a result of specified decay processes of selected molecular or fragmentation ions.

Conclusion

One of the important areas of chromatomass-spectrometric o analysis is chemical analysis, in particular, trace analysis of potentially hazardous substances in the environment, food, biological fluids and tissues. As an example, the determination of polychlorinated dibenzo-1,4-dioxins and dibenzofurans with extreme toxicity can be given (the MPC for these compounds is 20 pg/l for water, 1-10 ng/kg for meat and fish products). To determine these compounds, only high- or low-resolution chromatography-mass spectrometry is used, mainly with electron impact ionization (sometimes negative chemical ionization and tandem mass spectrometry are used) and using the isotope dilution method. The analysis should ensure the absolute sensitivity of the determination of dioxins at a level not worse than 0.1 pg, while gas chromatographic separation of all ethers, dibenzodioxins and dibenzofurans, for which the values of toxicity equivalents are established, from other isomers and interfering compounds, the possibility of simultaneous registration of several (at least two) ions for each compound being determined is necessary.

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