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MASS SPECTROSCOPIC ANALYSIS OF BENZENE-1,4-DICARBONIC ACID

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Abstract. In this scientific work, we will get acquainted with the results of comparing the theoretical and practical results of the mass-spectroscopic analysis of benzene dicarboxylic acids belonging to the carboxyl group.

Key words. Aromatic dicarboxylic acids, substance, benzene, correction, phthalic acid, electrophilic, substitution, isophthalic acid, (IR), absorption mass-spektroskopik.

INTRODUCTION Mass spectrometry is a method of checking the mass of atoms and molecules in a substance based on their spectrum. Each substance whose atoms and molecules are ionized differs from each other in the t/ye ratio, which is measured by mass spectrometers. According to the obtained spectrum, the mass of the substance and the amount of other substances in the body are found. Mass spectroscopy is one of the main analytical methods in applied physics, chemistry, biology, medicine, geology and technology. There are different ways to determine the mass of matter in a body archive. Mass, the distance between the dispersion lines is determined by the doublet method, and the mass difference is found based on this distance. The mass of substances is determined by the method of measuring the ion current.

Mass spectroscopy is also used to determine gas composition. Gases are tested by total evaporation, isotope separation, vacuum sparking, and ion bombardment. A certain amount of substance is examined by mass spectroscopy, the amount of elements in it - the amount of components in gas mixtures is controlled and determined, and isotopes are obtained. In the chemical industry, technological processes are managed with mass spectroscopy, the structure of the upper atomic layer is studied, the processes of the collision of charged particles are observed, and the kinetics of chemical reactions are checked. Mass spectroscopy is the only method in many fields. The neutral and ionic composition of the Earth's upper atmosphere has been measured using mass spectroscopy, and the composition of other planets' atmospheres can also be measured in this way.

In the process of mass spectroscopic analysis of benzene-1,4-dicarboxylic acid, based on its molecular structure, a number of important mass spectrometric signals can be observed. Benzene-1,4-dicarboxylic acid ($C_8H_6O_4$) is a compound in the form of a benzene ring with two carboxyl groups.

Theoretical basis of molecular ion (M^+) and molecular mass point:

- Since its molecular formula is $C_8H_6O_4$, its molecular mass is approximately 166 g/mol.

- In the mass-spectroscopic spectrum, the peak of the molecular ion (M^+) can be seen around 166 amu (atomic mass units).

Benzene-1,4-dicarboxylic acid can be separated into different fragments during mass spectrometric analysis. The main fragmentations include:

- In the process of decarboxylation of the carboxyl group in the carbonic acid fragment, the CO_2 molecule can be separated. This reaction is visible in mass spectroscopy as 166 → 146 amu ($M^+ \rightarrow M^+ - CO_2$).

- In the phenyl fragment, the benzene ring remains almost intact, and the fragment can appear in the form of 120 amu ($C_6H_6^+$). This fragmentation is related to the separation of the carboxyl group.

The main pixels that can be seen in the mass spectroscopic spectrum:

M^+ (166 amu)

$M^+ - CO_2$ (146 amu)

$M^+ - C_6H_6$ (120 amu)

$M^+ - CO$ (28 amu)

Isotopic peaks (167, 168 amu)

CONCLUSION

Mass spectroscopic analysis of benzene-1,4-dicarboxylic acid helps to confirm the presence of the benzene ring and carboxyl group through its molecular mass and fragmentation. The indicated fragments and masses are useful in determining the structural properties of this compound.

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