IR-SPECTROSCOPIC, MASS-SPECTROSCOPIC ANALYSIS OF BENZENE-1,4-DICARBOXYLIC ACID, A REPRESENTATIVE OF AROMATIC DICARBOXYLIC ACIDS

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

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

Аннотация. В данной научной работе мы познакомимся с результатами сопоставления теоретических и практических результатов масс-спектроскопического и ИК-спектроскопического анализа бензолдикарбоновых кислот, относящихся к карбоксильной группе.

Ключевые слова. Ароматические дикарбоновые кислоты, абсорбция, вещество, бензол, коррекция, фталевая кислота, электрофильный, замещение, изофталевая кислота, (ИК), абсорбционная масс-спектроскопия.

INTRODUCTION. The basic principle of IR spectroscopy is that when a molecule absorbs infrared light, its atoms and bonds perform different vibrations. These vibrations are divided into types such as Stretching (changing length) and Bending (bending).

The main features of IR spectroscopy are vibrations and spectral lines: In IR spectroscopy, each absorption line in the spectrum reflects the vibrations of different bonds in the molecule. The spectrum contains information that indicates which line absorbs which amount of energy.

Benzene-1,4-dicarboxylic acid ($C_6H_4(CO_2H)_2$) molecule consists of an aromatic ring with both carboxyl (-COOH) groups in positions 1 and 4 of the benzene ring. IR spectroscopy helps in analyzing the structure and functional groups of this molecule.

Aromatic Ring Absorptions The C-H bonds in the benzene ring produce broad and detectable absorptions visible in the infrared spectrum. These are usually:

- Aromatic C-H absorptions: Strong, indistinct bands appear around 3000 cm^{-1}. These lines correspond to the C-H bonds in the aromatic ring.

- Aromatic C=C absorptions: There are weak and strong absorptions between 1450 cm^{-1} and 1600 cm^{-1}. These lines arise from the vibrations of the C=C bonds in the aromatic system.

LITERATURE ANALYSIS AND METHODOLOGY

In the absorption of the carboxyl (-COOH) group, the absorption of two carboxyl groups in the molecule of benzene-1,4-dicarboxylic acid plays an important role in the IR spectrum:

- C=O absorption: a strong and defined line appears around 1700 cm^{-1}. This indicates that the carboxyl group is a carbonyl (C=O) bond. The strength of absorption can depend on the crystalline state of the acid or its liquid state.

- O-H absorption: broad and weak absorption lines appear between 2500-3300 cm^{-1}. These lines arise from hydrogen bonds and are characteristic of the carboxyl group. This absorption may be stronger if the molecule is hydrogenated.

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.

RESULTS. 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 ($M^+ \rightarrow M^+ - CO_2$).

CONCLUSION

Mass spectroscopic analysis of benzene-1,4-dicarboxylic acid helps confirm the presence of the benzene ring and carboxyl group through its molecular mass and fragmentation. The indicated fractions and masses are used to determine the structural properties of this compound. IR spectroscopic analysis of benzene-1,4-dicarboxylic acid helps to determine the presence of functional groups of the molecule and interactions between them.

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