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IR SPECTROSCOPIC ANALYSIS OF BENZENE-1,4-DICARBOXYLIC 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 infrared spectroscopic analysis of benzene dicarboxylic acids belonging to the carboxyl group.

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

INTRODUCTION Infrared (IR) spectroscopy is an analytical technique that studies the absorption of infrared light by substances and helps determine their molecular structure. The basic principle of IR spectroscopy is that molecules are exposed to infrared light and absorb their chemical bonds (vibrations) partially or completely as indicators of energy. This method is very useful in obtaining information about molecules and their functional groups.

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).

Each chemical bond and functional group (for example -OH, -NH2, -COOH) is characterized by its own absorption lines.

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.

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.

Additional spectral features, in turn, are divided into two types:

1). Narrow and broad absorptions of the aromatic ring- The spectrum of benzene-1,4-dicarboxylic acid shows a small and strong C=C absorption around 1600 cm^{-1} and a narrow absorption around 1500 cm^{-1}. These absorptions reflect the chemical environment of the aromatic system in the molecule.

2). Cross-bonds and transformations - hydrogen bonding of the O-H group and absorption of the C=O group can create different energy states in the molecule. This can vary in spectrum depending on whether the molecule is in a crystalline or liquid state.

CONCLUSION

IR spectroscopic analysis of benzene-1,4-dicarboxylic acid helps to determine the presence of functional groups of the molecule and interactions between them. Key features such as aromatic C-H absorption (3000 cm^{-1}), carboxyl group C=O absorption (1700 cm^{-1}) and O-H absorption (2500-3300 cm^{-1}) play an important role in identifying and characterizing this molecule. These lines in the IR spectrum help to fully understand the chemical structure and physical state of the molecule

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