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Chemical composition of Phenolphthalein determined by IR spectroscopy

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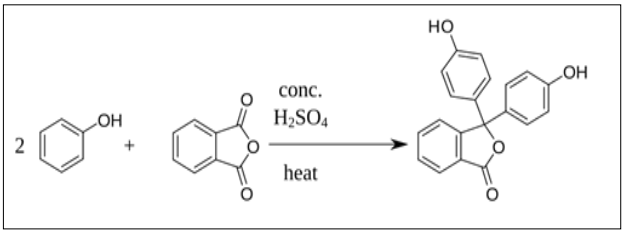
Abstract
In this article, we determined the composition of phenolphthalein by IR spectroscopy using a Shimadzu FTIR spectrometer. The wavenumber range is between 3300 and 500cm^{-1}. Phenolphthalein contains the following functional groups: O-H, C=O, C=C, C-C and aromatic compounds. Phenolphthalein is a widely used organic compound, notably as an acid–base indicator, whose chemical composition and functional groups can be effectively characterized by infrared (IR) spectroscopy. In this study, IR spectroscopic analysis was employed to determine and confirm the molecular structure of phenolphthalein. The IR spectrum exhibited characteristic absorption bands corresponding to its functional groups, including a broad band in the region of 3200–3600 cm^{-1} attributed to phenolic O–H stretching vibrations, strong absorptions near 1700–1750 cm^{-1} associated with the carbonyl (C=O) group of the lactone ring, and bands in the 1500–1600 cm^{-1} region corresponding to aromatic C=C stretching vibrations. Additional peaks observed between 1000–1300 cm^{-1} were assigned to C–O stretching vibrations. These spectral features are consistent with the known molecular formula ($C_{20}H_{14}O_4$) and structure of phenolphthalein. The results demonstrate that IR spectroscopy is a reliable and effective technique for identifying the chemical composition and confirming the functional groups present in phenolphthalein.

Keywords: Composition, IR spectrum, Phenolphthalein

Introduction

Phenolphthalein is a chemical substance that occurs as colorless white crystals, soluble in alcohols (methanol, ethanol, propanol, isopropanol, etc.) and less soluble in water. It is used, in particular, as a pH indicator in titrations. In the past, it was used in medicine as a purgative/laxative and as a hemoglobin indicator (Kastle-Meyer test) [1, 5].

Phenolphthalein can be synthesized by condensing phthalic anhydride with two molecules of phenol in the presence of concentrated H_2SO_4. The reaction can also be catalyzed by a mixture of zinc chloride and thionyl chloride.



In acidic medium it exists in the lactone form with the carbon of the triarylmethane skeleton sp^3 hybridized, with the electrons not participating in the conjugation with the aromatic nuclei. Under the action of alkaline solutions, it is transformed into a red disodium salt with a quinone structure. The carbon is sp^2 hybridized, as a result of which a conjugation with the aromatic nuclei takes place, the conjugation thus ensuring the stability of the color. Excess of a strongly alkaline solution causes the destruction of the structure and the disappearance of the color. At this stage, phenolphthalein passes into the carbinolic structure (since an alcohol called carbinol is obtained) and returns to the sp^3 hybridization of the central carbon [6, 12].

Medicine as a laxative, currently no longer used due to its carcinogenic potential. Kastle-Meyer test for highlighting blood. In titrimetry, along with its derivatives: Eosin, Timolftalein, Fluorescein.

Materials and methods

Materials

Analytical-grade phenolphthalein ($C_{20}H_{14}O_4$) was used without further purification. Potassium bromide (KBr), spectroscopic grade, was employed for pellet preparation. All materials were handled under dry conditions to prevent moisture interference in the infrared spectra.

Methods

The chemical composition of phenolphthalein was determined using infrared (IR) spectroscopy. A small quantity of finely powdered phenolphthalein (approximately 1–2 mg) was thoroughly mixed with dry KBr (about 100 mg) using an agate mortar and pestle to obtain a homogeneous mixture. The mixture was then compressed under high pressure to form a transparent KBr pellet.

The IR spectrum of the prepared pellet was recorded using a Fourier Transform Infrared (FTIR) spectrophotometer in the mid-infrared region, typically from 4000 to 400 cm^{-1}. A background spectrum of pure KBr was recorded prior to sample analysis to eliminate atmospheric and instrumental interferences.

The obtained IR spectrum was analyzed by identifying characteristic absorption bands corresponding to functional groups present in phenolphthalein. The observed peaks were compared with standard reference spectra and literature values to confirm the chemical composition and structural features of the compound.

Fourier transform infrared (FT-IR) spectral analysis of phenolphthalein indicator was performed. Various functional groups present in phenolphthalein were recorded in the form of FT-IR (ATR) spectra using Shimadzu FTIR spectrometer in the range of 4000–400 cm^{-1}.

Fig 1: Shimadzu FTIR spectrometer

Result and discussion

The infrared (IR) spectrum of phenolphthalein exhibited several characteristic absorption bands that confirm its chemical composition and molecular structure. A broad absorption band observed in the region of 3200–3600 cm^{-1} is attributed to the O–H stretching vibrations of the phenolic hydroxyl groups, indicating the presence of hydrogen-bonded –OH functionalities.

A strong and sharp absorption band appeared around 1700–1750 cm^{-1}, which corresponds to the C=O stretching vibration of the lactone carbonyl group, a key structural feature of phenolphthalein. The presence of this peak confirms the lactone form of the molecule under neutral conditions.

Absorption bands in the range of 1500–1600 cm^{-1} were assigned to aromatic C=C stretching vibrations, reflecting the benzene ring structures present in phenolphthalein. Additional medium-intensity peaks observed between 1000 and 1300 cm^{-1} are due to C–O stretching vibrations of the phenolic and ester groups. Weak bands detected in the region of 700–900 cm^{-1} correspond to out-of-plane C–H bending vibrations of substituted aromatic rings.

The overall IR spectral pattern closely matches reported reference spectra for phenolphthalein, confirming its molecular formula ($C_{20}H_{14}O_4$) and functional group composition. The results demonstrate that IR spectroscopy is an effective technique for identifying and verifying the chemical composition and structural characteristics of phenolphthalein.

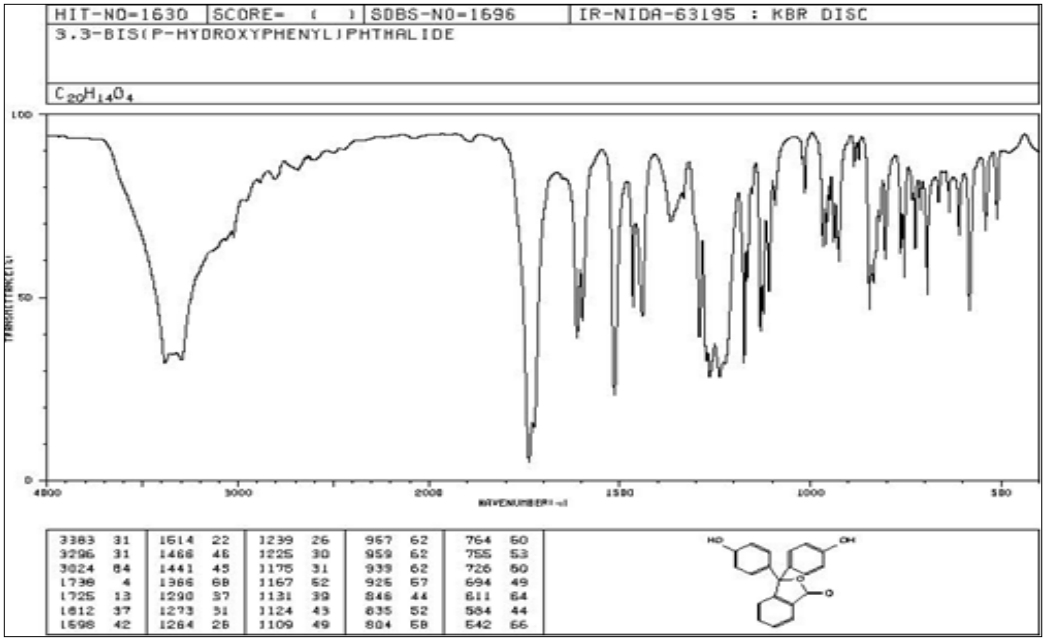


Fig 2: Spectrul IR al fenolftaleinei

It was observed that the phenolphthalein indicator exhibits a sharp band between 3300 and 3500 cm^{-1} revealing the the phenolic C=O group. Additionally, C=O stretching (essential band in phenolphthalein) was observed at 1700 cm^{-1}. Interestingly, there was a sharp intense band at 1030 cm^{-1} revealing the presence of aromatic ring breatingh (fig.2) [13, 17].

Table 1 shows the assignment of peaks in the FTIR spectrum of phenphthalein.

Table 1: Peak assignment in the FTIR spectrum of phenolphthalein

Wave number, cm^{-1}	Functional grouping	Vibration mode
3300	O-H	stretch
1700	C=O	stretching
1600	C=C	stretching
1670	C-C	stretching
500-1000	flavored	Ring breathing

Conclusion

The wavenumber range is between 4000 and 500cm^{-1}. Phenolphthalein contains the following functional groups: O-H, C=O, C=C, C-C and aromatic compounds and were determined with the Shimadzu FTIR spectrometer. Infrared (IR) spectroscopic analysis successfully confirmed the chemical composition and structural features of phenolphthalein. The presence of characteristic absorption bands corresponding to phenolic O–H, lactone carbonyl (C=O), aromatic C=C, and C–O functional groups is consistent with the known molecular structure and formula ($C_{20}H_{14}O_4$) of phenolphthalein. The close agreement between the observed IR spectrum and reported reference data demonstrates the reliability of IR spectroscopy as a simple and effective method for identifying phenolphthalein and verifying its functional group composition. This study highlights the usefulness of IR spectroscopy in qualitative

chemical analysis and structural characterization of organic compounds.

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