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# Composition of polystyrene determined by IR spectroscopy

**Ioana Stanciu**
Department of Physical Chemistry, Faculty of Chemistry,University of Bucharest, Bucharest, Romania

## Abstract

Fourier transform infrared spectroscopy (FTIR) is a fundamental analytical technique for characterizing the chemical structure of polymers, including polystyrene. Spectroscopic analysis reveals the presence of specific absorption bands, which confirm the existence of aromatic phenyl units attached to the polymer chain. The characteristic spectrum of polystyrene highlights the following main regions: 3100–3000 $cm^{-1}$ (aromatic C–H stretching vibrations), 3000–2850 $cm^{-1}$ (aliphatic C–H stretching vibrations), 1600–1490 $cm^{-1}$ (aromatic ring C=C stretching bands), 1450–1370 $cm^{-1}$ (C–H bending vibrations), 1025–1000 $cm^{-1}$ (in-plane C–H vibrations) and 750–690 $cm^{-1}$ (monosubstituted C–H out-of-plane deformation bands). These spectral signatures confirm the chemical structure of polystyrene and allow its differentiation from other styrene-based polymers or copolymers. At the same time, FTIR is a useful tool not only for material identification, but also for monitoring degradation, oxidation or chemical functionalization processes, providing relevant information in the field of materials science and polymer recycling.

**Keywords:** chemical composition, polystyrene, IR spectroscopy

## Introduction

Polystyrene is a polymeric material, slightly transparent, amorphous or partially crystalline, thermally processable (thermoplastic). It is not an electrical conductor. It is made from styrene monomer, a simpler liquid hydrocarbon obtained from petroleum. Polystyrene is one of the most widespread types of plastic, with a (significant) global consumption of billions of kilograms per year.

Characteristics: solid at room temperature, processable by heating (thermoplastic), has a softening temperature of approximately 100 °C and returns to the solid state upon cooling, is used as an industrial (construction) material in solid or spongy (spongy) form [1-5].

The density of polystyrene is a measure of its mass per unit volume, usually expressed in kilograms per cubic meter ($kg/m^3$). Essentially, the density indicates how compacted the polystyrene granules are in a given volume. The higher the density of polystyrene, the better the material will have a thermal insulating capacity. A denser polystyrene has fewer air spaces between the granules, thus reducing heat transfer.

Density also influences the mechanical strength of polystyrene. A high-density polystyrene will be more resistant to compression and other mechanical stresses. For example, a high-density polystyrene is more suitable for use in applications that require structural support, such as under a concrete screed or under floors. High-density polystyrene is usually more dimensionally stable and more durable over time, being less susceptible to compression and deformation.

## Types of expanded polystyrene

EPS is the abbreviation for Expanded Polystyrene, and the number indicates its quality.

**EPS 50: Density:** Approximately 10-15 $kg/m^3$ Compressive strength: 50 kPa at 10% deformation Applications: Thermal insulation for roofs, facades and external walls, where high mechanical strength is not required.

**EPS 70: Density:** Approximately 15-20 $kg/m^3$ Compressive strength: 70 kPa at 10% deformation Applications: Thermal and acoustic insulation for walls, floors and roofs, with a lower load-bearing capacity.

**EPS 80: Density:** Approximately 18-20 $kg/m^3$ Compressive strength: 80 kPa at 10% deformation Applications: Insulation for walls, floors and roofs, offering a balance between thermal performance and mechanical resistance.

**EPS 100: Density:** Approximately 20-25 $kg/m^3$ Compressive strength: 100 kPa at 10% deformation Applications: Insulation for floors, roofs and walls requiring moderate mechanical resistance.

**EPS 120: Density:** Approximately 25-30 $kg/m^3$ Compressive strength: 120 kPa at 10% deformation Applications: Floors, terraces, basement walls or other surfaces requiring higher compressive strength.

**EPS 150: Density:** Approximately 30-35 $kg/m^3$ Compressive strength: 150 kPa at 10% deformation Applications: Insulation for foundations, under floors with heavy traffic, or in applications where a high load-bearing capacity is required.

**EPS 200: Density:** Approximately 35-40 $kg/m^3$ Compressive strength: 200 kPa at 10% deformation Applications: Industrial floors, floating screeds, or other structural applications where very high mechanical strengths are required.

**EPS 250: Density**: Approximately 40-45 $kg/m^3$ Compressive strength: 250 kPa at 10% deformation Applications: Infrastructure projects or constructions that require extremely high compressive strength [6-12].

In construction, the quality of polystyrene must be at least ESP100

## Materials and methods

Styrene ($C_8H_8$, chemically pure) was alternately washed six times with 0.1 mol/L NaOH and deionized water in order to remove the polymerization inhibitor.

Apparatus used were Fourier Transform Infrared (Perkin Elmer FT-IR Spectrophotometer Frontier).

**Fig.1:** Perkin Elmer FT-IR Spectrophotometer

## Results and discussions

Figure 2 illustrates the infrared absorption spectra of the polystyrene spheres whose average particle size is about 560 nm. Obviously, there are several absorption peaks within the involved wavenumber range. There are absorption peaks at the wave numbers of 3060.8 $\text{cm}^{-1}$ and 3026.0 $\text{cm}^{-1}$ due to aromatic C-H stretching vibration absorption and there are three absorption peaks at the wave numbers of 1600.8 $\text{cm}^{-1}$, 1492.7 $\text{cm}^{-1}$, and 1452.2 $\text{cm}^{-1}$ due to aromatic C=C stretching vibration absorption. These absorption peaks indicate the existence of benzene rings. The absorption peaks at the wave numbers of 756.0 $\text{cm}^{-1}$ and 698.2 $\text{cm}^{-1}$ correspond to C-H out-of-plane bending vibration absorption and indicate that there is only one substituent in the benzene ring. Figure 2 also shows the absorption peaks at the wave numbers of 2921.9 $\text{cm}^{-1}$ and 2848.6 $\text{cm}^{-1}$, corresponding to the existence of methylenes.

These IR results have confirmed that the styrene reacts to produce polystyrene through polymerization reaction. In addition, the absorption peaks at the wave number of 3446.5 $\text{cm}^{-1}$ is for the stretching vibration absorption of O-H, which indicates the existence of hydroxyl. The hydroxyl may come from water or hydrolysis of strong acid weak alkali salt such as sodium p-styrenesulfonate, potassium hydrogen carbonate [13-19].

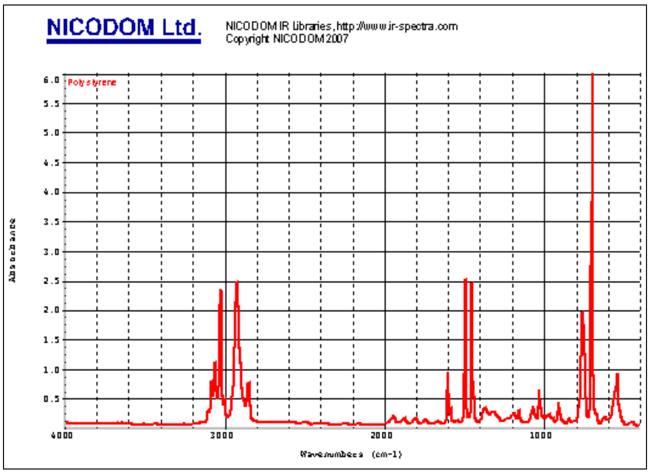

**Fig.2:**. Spectrul IR al polistirenului

## Conclusions

FTIR spectroscopic analysis confirmed the specific chemical structure of polystyrene by identifying bands characteristic of both the aromatic chain and the aliphatic segments. The presence of aromatic C–H stretching vibrations (3100–3000 $\text{cm}^{-1}$), of the C=C bands of the phenyl ring (1600–1490 $\text{cm}^{-1}$) and of the C–H “out of plane” deformations (750–690 $\text{cm}^{-1}$) constitute clear evidence of the existence of monosubstituted phenyl units attached to the polymer chain. Also, the aliphatic bands in the 3000–2850 $\text{cm}^{-1}$ region confirm the hydrocarbon structure of the polymer backbone. Therefore, FTIR proves to be an effective method for identifying polystyrene and differentiating it from other polymers, as well as for monitoring structural changes occurring following degradation, recycling or chemical functionalization processes.

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