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Chemical composition of aromatic organic compounds with condensed nuclei

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Abstract

Polycyclic aromatic hydrocarbons (PAHs) are a class of organic compounds with two or more condensed aromatic rings, with specific structures, persistent in the environment and with varied toxicity.

In this article we determined by FTIR the chemical composition of aromatic compounds with condensed rings: naphthalene, anthracene and phenanthrene. The FTIR spectra of the 3 compounds were determined with a Bruker spectrophotometer between 4000 and 375 cm^{-1}, with resolution of 4 cm^{-1}.

Keywords: Aromatic compounds, naphthalene, anthracene, phenanthrene

Introduction

Polycyclic aromatic hydrocarbons (PAHs) are a class of organic compounds with two or more condensed aromatic rings, with specific structures, persistent in the environment and with varied toxicity. Hundreds of PAHs have been released into the environment, from both anthropogenic processes (incomplete combustion/pyrolysis of organic matter), natural processes (burning of vegetation/wood, volcanic eruptions) and biological processes of biosynthesis/biodegradation of organic matter. Because PAHs have been detected in air, soil, water and biological processes occur everywhere in nature, PAHs are considered ubiquitous in the environment. [1-3].

Polycyclic aromatic hydrocarbons (PAHs) are formed by pyrogenic, petrogenic and biological processes. Pyrogenic PAHs are formed when organic matter is exposed to high temperatures (3500C -12000C), in the absence of oxygen or in the presence of reduced amounts of oxygen. Examples of pyrogenic processes: thermal cracking of petroleum residues with the formation of light hydrocarbons, coal distillation, incomplete combustion of fuels in heating systems, in vehicle engines, incomplete combustion of forest wood, in heating systems, etc. Pyrogenic PAHs in high concentrations exist in emissions resulting from urban areas and near important sources of PAHs (industrial processes, including energy generating ones, incineration processes, etc.). Pyrogenic PAHs in low concentrations come from emissions resulting from transport activities (vehicles, airplanes, etc.), smoking, wood-burning stoves, activated sludge from water treatment plants, etc. [4].

Incomplete combustion, both natural and anthropogenic, is the largest contributor of PAHs in the environment [5]. Petrogenic PAHs are represented by crude oil, formed over millions of years, at low temperatures (100-1500C), but also PAHs formed during the transportation, storage and use of crude oil or petroleum products, the accumulation of small amounts of oil, gasoline, motor oils and substances associated with transportation activities, etc. Natural sources of PAHs are represented by the processes of burning wood/forest vegetation, volcanic eruptions, bacterial or algal syntheses, oil exploitation and biomass decomposition [6, 7]. Stationary sources produce approx. 80% of total PAH emissions; the rest of the emissions are produced by mobile sources (residues from the use of gasoline and diesel fuels, etc.). PAH emissions released in industrial production are less important, compared to PAHs resulting from incomplete combustion processes where closed systems and recycling processes are used. New heterocyclic aromatic compounds (carbazoles, acridines), as well as PAH derivatives (nitro-PAH and oxygenated PAHs) can be generated by incomplete combustion and by chemical reactions occurring in ambient air. These compounds occur together with PAHs in air, water and food, the total mixture being called polycyclic aromatic compounds (PAHs) [8]. Some PAHs are used as raw materials in the synthesis of some materials: - Acenaphthene: synthesis of pigments, dyes, plastics, pesticides, pharmaceuticals - Anthracene: diluent for wood bioprotection agents and synthesis of dyes and pigments - Fluoranthene: synthesis of chemicals used in agriculture, dyes, pharmaceuticals - Fluorene: synthesis of pharmaceuticals, pigments, dyes, pesticides and temperature-resistant plastics - Phenanthrene: synthesis of resins and pesticides - Pyrene: synthesis of pigments. The concern for reducing emissions of PAHs have been present since the 1950s, with the introduction of the first air pollution control policies. Currently, legislation on permissible PAH concentrations in the air, combined with legislation prohibiting the uncontrolled burning of industrial and agricultural waste, continues to contribute to reducing PAH concentrations in the air. However, in developing countries (China, India, Brazil, Sudan, etc.) where biomass and coal are the dominant sources of energy, PAH concentrations are still too high [9, 10].

Polycyclic aromatic hydrocarbons (PAHs) are a class of organic compounds with two or more linearly or angularly condensed benzene rings. Polycyclic aromatic hydrocarbon emissions to the atmosphere have a short or long transit time and can accumulate in wet or dry deposits. Depending on the number of benzene nuclei, PAHs are classified as:

- PAHs with low molecular weight are those that have less than 4 aromatic nuclei in their structure PAHs with high molecular weight have 4 or more aromatic nuclei in their structure PAHs with 2 or 3 nuclei (naphthalene, acenaphthene, anthracene, fluorene, phenanthrene) are present in the air, predominantly in the vapor phase PAHs with four nuclei (fluoranthene, pyrene, chrysene) exist in both the vapor and particulate states PAHs with 5 or more aromatic nuclei (benzo[g,h,i]perylene, etc.) are present predominantly in the particulate state Smaller molecules (benzene, toluene, naphthalene) are not considered true PAHs. The PAHs considered the most potent/potent carcinogens, and extensively studied, are 7,12-dimethylbenzoanthracene (DMBA) and benzo(a)pyrene (BaP) [11-13].

PAH compounds, in their pure state, are generally colored, solid, crystalline substances at ambient temperature [14]. The main characteristics of PAHs are their high melting and boiling points, low vapor pressure, and very low solubility in water. The physicochemical properties of PAHs vary considerably with their molecular weight and structure. The vapor pressure of PAHs decreases with increasing molecular weight and the solubility in water decreases with increasing molecular weight. The resistance to oxidation and reduction reactions also increases with molecular weight. PAHs are very lipophilic and therefore miscible with organic solvents [15]. The solubility in water decreases with each aromatic ring in the PAH structure and gives PAHs high mobility in the environment, storage, re-volatility and their distribution in air, soil and water. A significant percentage of PAHs is transported through the atmosphere over long distances (LRAT). PAHs released into the atmosphere are found in two separate phases, a vapor phase and a solid phase in which PAHs are adsorbed on particulate matter. PAHs also exhibit light sensitivity, heat resistance, corrosion, and physiological activity [16,17].

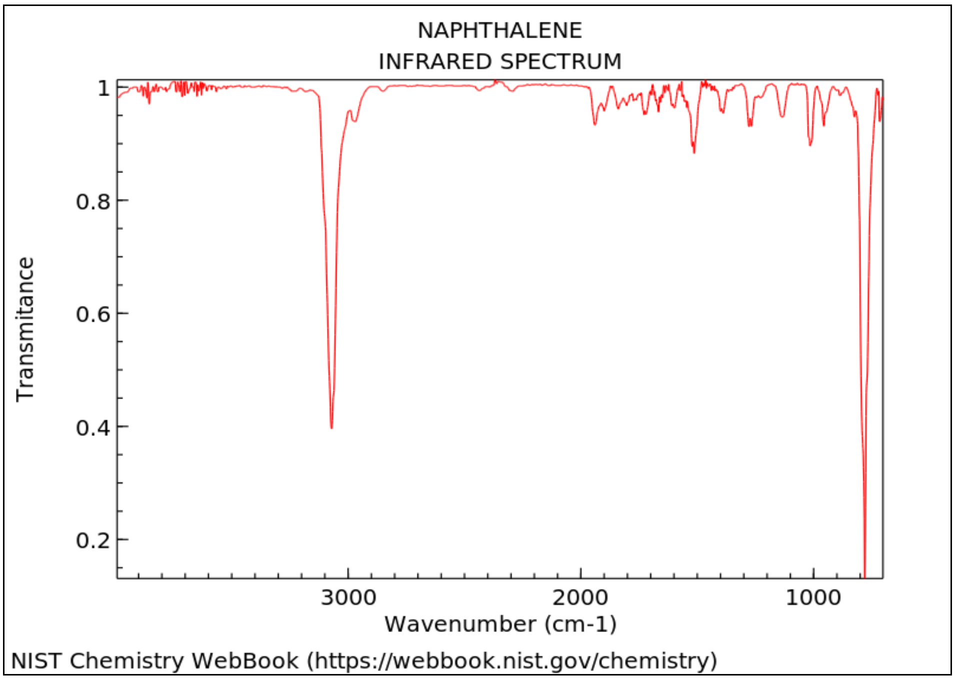
Material and methods

FT-IR spectrum were accomplished and recorded with Fourier-Transform infrared spectrophotometer (Bruker , Alpha ATR) between 4000 and 375 cm^{-1}, with resolution of 4 cm^{-1}.

Fig 1: Infrared spectrophotometer Bruker

Results and discussion

Figure 2 shows the FTIR spectrum of naphthalene.



NIST Chemistry WebBook (https://webbook.nist.gov/chemistry)

Fig. 2 Spectre FTIR of naphtalene

As we saw in the brief introduction to infrared spectroscopy, aromatic rings show a characteristic C-H stretching absorption at 3030 cm^{-1} and a series of peaks in the 1450 to 1600 cm^{-1} range of the infrared spectrum. The C-H bond stretching of all hydrocarbons occurs in the range of 2800-3300 cm^{-1}, and the exact location can be used to distinguish between alkane, alkene and alkyne. Specifically: ≡C-H (sp C-H) bond of terminal alkyne gives absorption at about 3300 cm (fig.2).

Figura 3 prezinta spectrul FTIR al antracenului.

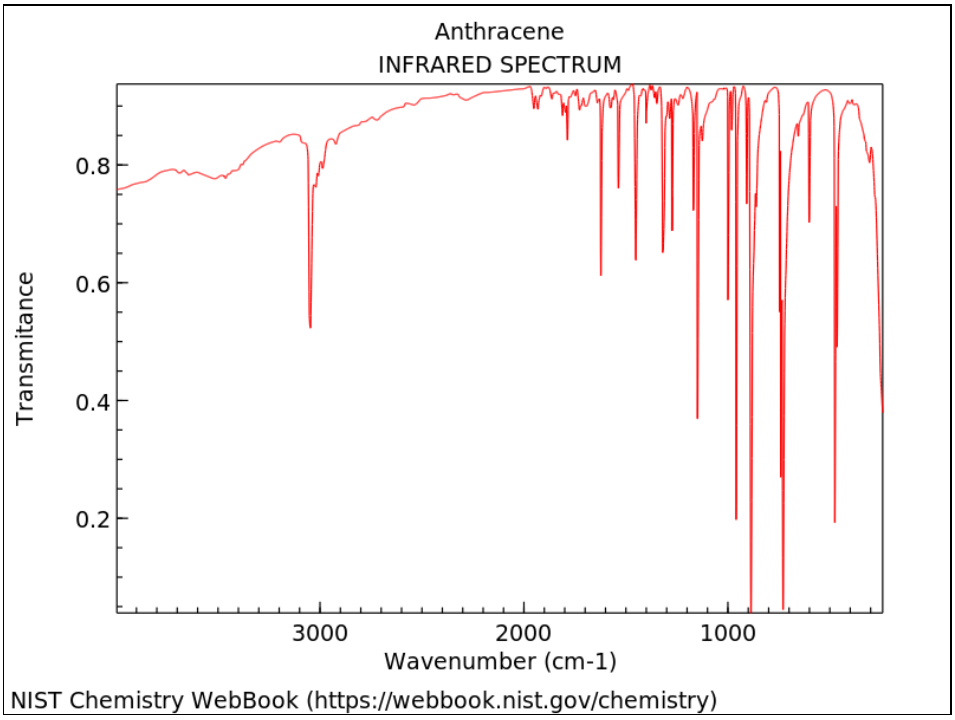


Fig 3: Spectre FTIR of antracene

We can divide the IR spectra into four regions, roughly 4000-2800, 2800-1900, 1900-1200, and 1200-400 cm^{-1}. The first region, above 2800, is characteristic of X-H bonds, or bonds to hydrogen. Triple bonds come at slightly lower frequency, followed by double bonds, and finally single bonds (Fig.3).

Figure 4 shows the FTIR spectrum of phenanthrene.

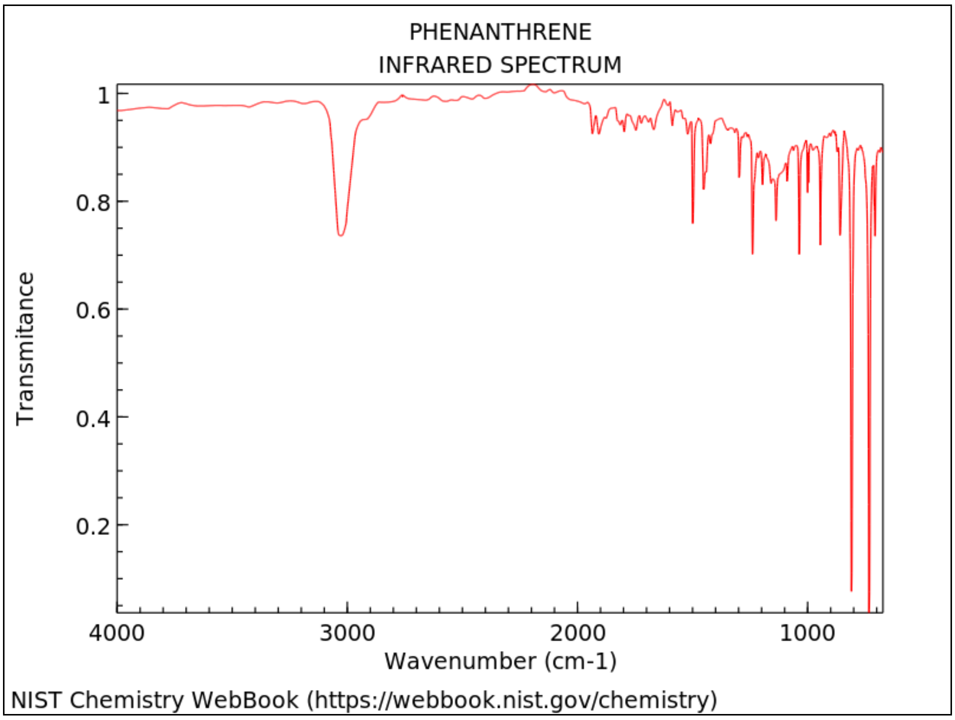


Fig 4: Spectre FTIR of phenanthrene

Phenanthrene ($C_{14}H_{10}$) is one of several PAHs that have a vibrational band at 3200-450 cm^{-1}.

We can divide the IR spectra into four regions, roughly 3200-2900, 2000-1700, 1750-1450, and 1500-1200 cm^{-1}, 1250-950 cm^{-1}, 1000-700 cm^{-1} , 750-450 cm^{-1} The first region, above 2800, is characteristic of X-H bonds, or bonds to hydrogen. Triple bonds come at slightly lower frequency, followed by double bonds, and finally single bonds.

Conclusions

In this article, we determined the chemical composition of the condensed ring aromatic compounds: naphthalene, anthracene and phenanthrene by FTIR with a Bruker spectrometer. The FTIR spectra of the 3 compounds naphthalene, anthracene and phenanthrene range between 4000 and 375 cm^{-1}, with a resolution of 4 cm^{-1}.

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