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# Evaluation And Investigation of Polycyclic Aromatic Hydrocarbons (PAH) in Liquid Sample: Impurity study

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***Abstract:*** Polycyclic aromatic hydrocarbons (PAHs) are a group of toxic organic compounds commonly found in liquid samples, including beverages, milk, fruit juices, and water, as well as in various food products. These compounds arise from combustion processes and environmental pollution, making it essential to monitor their levels in consumable liquids to mitigate potential health risks, including carcinogenic and developmental toxicity. This study investigates PAH concentrations in diverse liquid samples, such as tea (15 + 1 EU PAHs at 140°C), milk (16 US EPA PAHs), alcoholic beverages (beer, wine, spirits, with a PAH value of 16 US EPA PAHs), and fresh fruit juices (apple, mango, orange, peach, pineapple at 0.2 g/L US EPA PAHs). Water sources, including tap water, river water, and normal water, were also assessed for trace PAH contamination.

Given the complexity of PAH mixtures in liquid samples, precise and sensitive analytical techniques are required to identify and quantify these compounds accurately. Gas chromatography-mass spectrometry (GC-MS) is frequently used for PAH analysis in liquid samples due to its high sensitivity, accuracy, and ability to separate complex mixtures.

***Keywords:*** *PAH, GC-MS, accuracy, liquid samples.*

## INTRODUCTION

Polycyclic aromatic hydrocarbons (PAHs) are organic compounds that are mostly colorless white or pale-yellow solids. They are a ubiquitous group of several hundred chemically related compounds, environmentally persistent with various structures and varied toxicity. They have toxic effects on organisms through various actions. Generally, PAHs enter the environment through various routes and are usually found as a mixture containing two or more of these compounds, e.g. soot. Some PAHs are manufactured in the industry. The mechanism of toxicity is considered to be interference with the function of cellular membranes as well as with enzyme systems which are associated with the membrane. It has been proved that PAHs can cause carcinogenic and mutagenic effects and are potent immune suppressants. Effects have been documented on immune system development, numeral immunity and on host resistance. PAHs can be formed both during biological processes and as products of incomplete combustion from either natural combustion sources (forest and brush fires) or man-made combustion sources (automobile emissions and cigarette smoke). Thus, PAHs are commonly detected in air, soil, and water. Therefore, PAHs are considered ubiquitous in the environment [1-2].

The term PAH refers to compounds consisting only carbon and hydrogen atoms. Chemically the PAHs are comprised of two or more benzene rings bonded in linear, cluster, or angular arrangements. Such molecular arrangements are illustrated in. Although there are many PAHs, most regulations, analyses and data reporting focus on only a limited number of PAHs, typically between 14 and 20 individual PAH compounds. Polycyclic aromatic hydrocarbons have two or more single or fused aromatic rings with a pair of carbon atoms shared between rings in their molecules [3].

**TPYES OF PAH:**

- Naphthalene - Two fused benzene rings.
- Anthracite - Three fused benzene rings in a linear arrangement.
- Phenanthrene - Three fused benzene rings in a non-linear arrangement.
- Pyrene-Four fused benzene rings in a linear arrangement
- Benzo[a]pyrene - Five fused rings with a specific arrangement, known for its carcinogenic properties
- Fluorene - Three rings with a fused benzene and a central cyclohexane
- Chrysene - Four fused benzene rings with a central anthracene structure.
- Benz[a̦]anthracene - Four rings with a structure similar to anthracene but with an additional benzene ring
- Dibenz[a,h]anthracene - Five fused rings with a structure that includes anthracene and an additional benzene ring,
- Benzo[b]fluoranthene - Five rings with a structure including two fused benzene rings and a central fluoranthene structure.
- Indeno[1,2,3-cd] pyrene - A complex structure with five fused rings that includes both pyrene and indene,
- Benzo[k]fluoranthene - Five fused rings with a specific arrangement involving F rings and fluoranthe [4-5].

**Advantages:**

**Energy storage and transmission:** PAHs are used in batteries, capacitors, and electrical conductors due to their excellent charge transport properties.

**Organic electronics:** PAHs are used in organic light-emitting diodes (OLEDs), organic photovoltaics (OPVs), and organic field-effect transistors (OFETs) due to their semiconducting properties.

**Dyes and pigments:** PAHs are used as colorants in inks, paints, and plastics due to their vibrant colors and stability.

**Pharmaceutical applications:** Some PAHs have been used as intermediates in the synthesis of drugs, such as antiviral and anticancer agents.

**Materials science:** PAHs are used as building blocks for advanced materials, such as graphene, nanotubes, and supramolecular assemblies.

**Research and development:** PAHs are used as model compounds in scientific research, helping to understand chemical reactions, molecular interactions, and environmental processes.

**Industrial applications:** PAHs are used in the production of lubricants, fuels, and coatings due to their chemical stability and performance.

**Catalysis:** PAHs are used as catalysts in various chemical reactions, such as hydrogenation, dehydrogenation, and oxidation.

**Environmental remediation:** Certain PAHs can be used to clean up contaminated soil and groundwater due to their ability to bind to pollutants.

**Cosmetics:** Some PAHs are used in cosmetics and personal care products, such as hair dyes, skin care products, and fragrances.

**Agriculture:** PAHs are used in pesticides, herbicides, and fungicides due to their biological activity.

**Biomedical applications:** PAHs have been explored for use in biomedical applications, such as drug delivery, imaging, and diagnostics.

**Nanotechnology:** PAHs are used as building blocks for nanomaterials, such as nanotubes, nanowires, and nanoparticles.

**Optoelectronics:** PAHs are used in optoelectronic devices, such as photodetectors, phototransistors, and optical sensors.

**Sensing applications:** PAHs are used as sensing materials for detecting various analytes, such as gases, ions, and biomolecules.

**Supramolecular chemistry:** PAHs are used to create supramolecular assemblies, which have potential applications in materials science and nanotechnology.

**Theoretical chemistry:** PAHs are used as model compounds to study chemical reactions, molecular interactions, and quantum mechanics.

**Astrochemistry:** PAHs are found in interstellar space and are studied to understand the formation and evolution of galaxies [6].

**Disadvantages:**

**Bioaccumulation:** PAHs can accumulate in living organisms, potentially causing harmful effects.

**Toxicity:** PAHs can be toxic to humans and wildlife, even at low concentrations.

**Air and water pollution:** PAHs can contribute to air and water pollution, negatively impacting human health and the environment.

**Soil contamination:** PAHs can contaminate soil, affecting plant growth and ecosystems.

**Health effects:** Exposure to PAHs has been linked to various health problems, including respiratory issues, skin irritation, and reproductive problems.

**Neurotoxicity:** Some PAHs have been shown to be neurotoxic, affecting brain development and function.

**Endocrine disruption:** PAHs can interfere with hormone systems, potentially causing developmental and reproductive issues.

**Climate impact:** PAHs can contribute to climate change by absorbing solar radiation and influencing cloud formation.

**Food contamination:** PAHs can contaminate food, particularly grilled or smoked foods, posing a risk to human health.

**Occupational exposure:** Workers in industries that handle PAHs, such as mining or construction, may be at risk of exposure [7].

**Side Effects:**

**Human Health:** Cancer: PAHs are known carcinogens, linked to lung, skin, bladder, and other types of cancer.

Respiratory problems: Exposure to PAHs can cause respiratory issues, such as bronchitis, asthma, and chronic obstructive pulmonary disease (COPD).

Skin irritation: PAHs can cause skin irritation, including redness, itching, and dermatitis.

Eye irritation: Exposure to PAHs can cause eye irritation, including conjunctivitis and cataracts.

Neurological problems: PAHs can affect the nervous system, leading to headaches, dizziness, and neurological damage.

Reproductive issues: Exposure to PAHs has been linked to reproductive problems, including birth defects and infertility.

Immune system suppression: PAHs can weaken the immune system, making people more susceptible to infections.

**Environmental:**

1. Water pollution: PAHs can contaminate water sources, harming aquatic life.

2. Soil pollution: PAHs can persist in soil, affecting plant growth and ecosystems.

3. Air pollution: PAHs can contribute to air pollution, negatively impacting human health and the environment.

4. Bioaccumulation: PAHs can accumulate in wildlife, potentially causing harmful effects.

5. Climate impact: PAHs can contribute to climate change by absorbing solar radiation and influencing cloud formation.

**Other:**

1. Food contamination: PAHs can contaminate food, particularly grilled or smoked foods.

2. Occupational exposure: Workers handling PAHs may experience exposure-related health issues.

3. Environmental persistence: PAHs can persist in the environment for long periods, causing ongoing harm [8-9].

**LIQUID SAMPLE AND PAH:**

Polycyclic aromatic hydrocarbons (PAHs) are a group of organic compounds composed of multiple fused aromatic rings. These compounds are of significant environmental and health concern due to their persistence, bioaccumulation, and potential carcinogenicity. PAHs can be found in various environmental matrices, including air, soil, and water, and can also contaminate food and beverages. River water is a crucial resource that supports a wide range of ecological, agricultural, and human activities. However, it is vulnerable to contamination from various sources, including industrial discharges, agricultural runoff, urban waste, and atmospheric deposition. One significant class of pollutants found in river water is polycyclic aromatic hydrocarbons (PAHs). PAHs in river water are concerning because they can affect both aquatic life and human health. PAHs tend to bind with sediments, where they can persist for long periods, posing a threat to benthic organisms. These compounds can bio-accumulate in the food chain, leading to higher concentrations in fish and other aquatic organisms that may be consumed by humans.

Exposure to PAHs is associated with various health risks, including cancer, immune system suppression, and developmental effects. Therefore, the presence of PAHs in river water is closely monitored by environmental protection agencies. The detection and quantification of PAHs in river water are typically performed using advanced analytical techniques such as gas chromatography-mass spectrometry (GC-MS). Regular monitoring helps to ensure that PAH levels remain within safe limits set by regulatory agencies. Cleanup efforts, pollution control, and the enforcement of environmental regulations are essential to reducing PAH contamination in river systems Polycyclic aromatic hydrocarbons (PAHs) are a group of organic compounds composed of multiple aromatic rings. They are primarily formed through incomplete combustion of organic materials, such as coal, oil, gas, wood, and other organic substances. PAHs are known for their potential health risks, including carcinogenicity, mutagenicity, and toxicity [10-11].

| **Sample** | **PAH** | **Sample treatment and preparation** | **Analytical instrument; column (column dimension)** | **Oven temperature program** | **Injection mode/ temperature** | **LOD (LOQ)** | **Percentage recovery (%)** | **Article** |
|---|---|---|---|---|---|---|---|---|
| TEA | 15+1 EU PAHs | PLE (acetonitrile and hexane) followed by GPC and SPE | Fast-GC/HRMS (10m×0.1mm,0.1µm | 140°C (1min) | Spitless (320°C) | 0.01-0.02µg/kg | 75-117 % | 18 |
| MILK | 16 US EPA PAHs | Saponification carried out in LLE, then mix dichloromethane and n-hexane (4:1, v/v) and purification of the organic layers | GC-MS; HP-5MS (30m×5mm,0.25µm | 65°C (1min) | N/A | N/A | 80-120% | 7 |
| **Beverage:** (a)beer (b)wine (c)spirits | 16 US EPA PAHs | Concentrated and cleanup using semi-automated SPE [packed with 60mg of silica-reversed phase with octadecyl functional groups (RP-C18) | GC-MS; DB-5MS (30×0.25mm×0.25mm) | 70°C (2min) | Spitless (320°C) | 0.02-0.6ng/L | 90-103% | 19 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Fresh juice: Apple Mango Orange Peach Pineapple** | US EPA (0.2 µg/L) | **Three key phases are included:** 1.sample cleanup 2.PAH analyte adsorption from fruit juice 3.desortion of PAH compound from the magnetic adsorbent | The specification of the GC-MS device, column and other condition | 65°C (1min) | N/A | 0.005-10µg/L | 94.8-102.4 % | 21 |
| **Water: Tap water River water** | 16 US EPA PAHs | Dispersive liquid-liquid micro-extraction solidification of floating organic droplet | gas chromatography–mass spectrometry (GC-MS) | The column temperature was initially held at 50 ◦C for 1 min, then increased to 200 ◦C at 15 ◦C/min, held for 5 min, and finally increased to 290 ◦C at 10 ◦C/min and held for 1 min. | freezer at −20 ◦C for 5 min | 0.0035-0.0141 µg/L | 93.8-105.2 % | 20 |

**What is Gas Chromatography-Mass Spectroscopy (GC-MS):**

Gas Chromatography-Mass Spectroscopy (GC-MS) is a powerful analytical technique used to separate, identify, and quantify the components of a mixture. It combines the separation capabilities of gas chromatography (GC) with the detection capabilities of mass spectrometry (MS) [12].

**Principles of GC-MS**

The GC-MS instrument consists of three main components:

- **Gas Chromatograph (GC):** The GC separates the components of a mixture based on their boiling points, affinity for the stationary phase, and molecular weight.
- **Mass Spectrometer (MS):** The MS detects the separated components based on their mass-to-charge ratio.
- **Interface:** The interface connects the GC and MS components, allowing the separated components to be transferred to the MS for detection [13].

**Advantages of GC-MS**

GC-MS offers several advantages, including:

- **High sensitivity and selectivity:** GC-MS can detect and identify trace amounts of analytes in complex matrices.
- **Qualitative and quantitative analysis:** GC-MS can provide both qualitative and quantitative information about the analytes present in a sample.
- **Wide range of applications:** GC-MS can be used for a wide range of applications, including environmental monitoring, pharmaceutical analysis, and food safety testing [14].

**Liquid Samples**

GC-MS can be used to analyze liquid samples, including:

- **Aqueous samples:** Water, blood, urine, and other aqueous samples can be analyzed using GC-MS.
- **Organic solvents:** Liquid samples dissolved in organic solvents, such as methanol or acetone, can be analyzed using GC-MS.
- **Biological samples:** Biological samples, such as tissue extracts or biofluids, can be analyzed using GC-MS.
- GC-MS (Gas Chromatography-Mass Spectrometry) is frequently used for analyzing liquid samples due to its numerous advantages. Here are some reasons why GC-MS is a popular choice for liquid sample analysis [15].

**Sensitivity and Selectivity**

- **High sensitivity:** GC-MS can detect and quantify very small amounts of analytes in liquid samples.
- **High selectivity:** GC-MS can distinguish between closely related compounds, reducing interference and improving accuracy [16].

**Separation and Identification**

- **Efficient separation:** Gas chromatography separates compounds based on their boiling points and affinity for the stationary phase, allowing for efficient separation of complex mixtures.
- **Unambiguous identification:** Mass spectrometry provides a unique mass spectrum for each compound, enabling unambiguous identification of analytes [17].

**Versatility and Robustness**

**Wide range of applications:** GC-MS can be used for various liquid sample types, including biological fluids, environmental samples, and pharmaceuticals.

- **Robustness and reproducibility:** GC-MS is a robust technique that provides reproducible results, making it suitable for routine analysis and quality control.

**Liquid Sample Compatibility**

- **Direct injection:** Many liquid samples can be directly injected into the GC-MS system, eliminating the need for extensive sample preparation.
- **Compatibility with various solvents:** GC-MS can accommodate a wide range of solvents, including aqueous and organic solvents [18-19].

**Quantitation and Limit of Detection**

- **Accurate quantitation**: GC-MS provides accurate quantitation of analytes, even at low concentrations.

- **Low limit of detection:** GC-MS has a low limit of detection, allowing for the detection of trace amounts of analyte [20-21].

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