



# The Impact of Polycyclic Aromatic Hydrocarbons on Environment and Humans

**Zeinab Ali Mohammad**

Master's student, Department of Organic Chemistry, Ilam University, Iraq

\*Correspondence author: [bbaa94827@gmail.com](mailto:bbaa94827@gmail.com)

**Abstract.** This research seeks to define polycyclic aromatic compounds, which are chemical compounds consisting of fused aromatic rings that do not contain heteroatoms or substituents. Many of these compounds are known to be carcinogenic and are primarily produced through the incomplete combustion of carbon-containing fuels such as wood, coal, diesel, grease, and tobacco. Pure polycyclic aromatic compounds generally appear as colorless, white, or pale green solids that often develop a yellowish tint over time. These substances are commonly found in coal tar, crude oil, creosote, and tar deposits in industrial and urban environments. Despite their widespread occurrence and potential health risks, only a limited number of polycyclic aromatic compounds are utilized in industrial applications, including the manufacture of medicines, dyes, plastics, and pesticides. Furthermore, this research examines the distribution, persistence, and accumulation of these compounds in the environment, as well as their toxicological effects on human health, ecosystems, and long-term environmental sustainability.

**Keywords:** Carcinogenic compounds; Environmental impact; Human health; Incomplete combustion; Polycyclic aromatic compounds

## 1. INTRODUCTION

Some natural products extracted from plants, such as dyes and resins, were of unknown composition at the beginning of development of organic chemistry. However, they possessed unique properties and were characterized by their aromatic scent. For this reason, they were called aromatic compounds, to distinguish them from other odorless compounds. This name is from Greek word "aroma," concept fragrant scent. Term "aromatic" was used in the past for substances like ethers and aromatic aldehydes. This terminology was replaced after the discovery of many odorless benzene derivatives.

Aromatic compounds are organic hydrocarbon compounds, meaning they are composed of hydrogen and carbon atoms. However, what distinguishes them from the second class of hydrocarbon compounds, called aliphatic compounds (alkanes, alkenes, and alkynes), is... Aromatic compounds always contain one or more benzene rings, unlike aliphatic compounds, which lack benzene ring. Aromatic compounds are also more stable than aliphatic compounds.

These compounds have chemical property where the molecule forms ring-like structure. The ring is typically hexagonal, containing (6) bonded carbon atoms; each one also bonded to hydrogen atom. The simplest aromatic molecule is benzene, with the chemical formula  $C_6H_6$ .

### Definition:

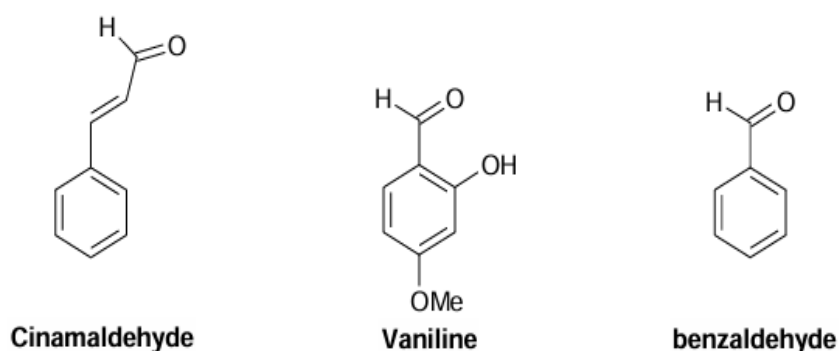
AC are defined as unsaturated hydrocarbon organic compounds that share a benzene ring. These are molecules that contain all carbon atoms. bonded together in single hydrocarbon

covalent bonds, and whose molecules contain at least one benzene ring, which is an unsaturated cyclic unit consisting of (6) carbon atoms known as the aromatic nucleus. Examples include benzene and phenol.



**Figure 1.** Phenol Benzene.

Many aromatic compounds are found in fragrant oils found in spices, fruits, and other parts of plants, such as bitter almond oil (enzaldehyde), cinnamon (cinnamaldehyde), and vanilla (vaniline).



**Figure 2.** Examples of aromatic compounds with aldehyde functional groups.

### Characteristics of Aromatic Compounds

It turned out that all that aromatic compounds share specific characteristics that distinguish them from aliphatic compounds. These characteristics include:

- 1) The aromatic compound contains ring made up of (6) called aromatic nucleus.
- 2) It does not react by addition and is not easily reduced, despite the presence of double bonds.
- 3) It is characterized by substitution reactions.
- 4) The aromatic compound is not easily oxidized unless it contains a side ring.
- 5) The presence of aromatic ring affects the properties of active groups to which it is attached.

## 2. TYPE OF AROMATIC COMPOUNDS

### Monocyclic Aromatic Compounds

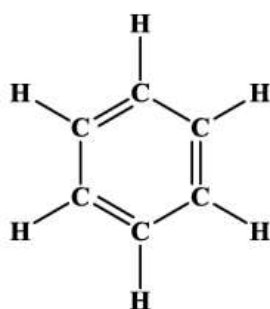
Organic compounds containing single flat ring of carbon atoms with delocalized pi electron cloud. The most well-known example is benzene (C<sub>6</sub>H<sub>6</sub>), which has hexagonal ring and unique properties. These compounds are highly stable and obey Hückel's rule. Their main characteristics include:

- 1) Single flat ring: Consists of single, flat ring of atoms.
- 2) Delocalized pi electron system: Double and single bonds alternate, but the electrons are not concentrated in one place and move freely around the ring, providing great stability.
- 3) Huckle rule: The number of  $\pi$  electrons in the ring must be followed Huckle rule, where it equals  $(4n + 2)$ , that (n) is positive integer. This rule is used to determine aromaticity.
- 4) Stability: They exhibit greater resistance to chemical reactions compared to alkenes due to stability of delocalized electron system.

Examples of monocyclic aromatic compounds include:

#### ***Benzene***

Benzene is the simplest parent aromatic compound. It was isolated in 1825 by Faraday from illuminating gas, which was used for lighting. In 1834, the initial formula for this compound was found to be (CH), and later the molecular formula was determined to be (C<sub>6</sub>H<sub>6</sub>). Several structural forms of benzene were proposed during these years, but these proved incorrect until correct form of benzene was proposed in 1865 by German scientist Kekulé. Therefore, benzene in this form is usually called Kekulé benzene.



**Figure 3.** Benzene.

Benzene contains six carbon atoms and six hydrogen atoms, with the formula C<sub>6</sub>H<sub>6</sub>. The benzene molecule has planar shape and contains successive system of  $\pi$  bonds (aromatic system). In the benzene molecule, each carbon atom is bonded to one hydrogen atom. It is customary to write the structural formula of benzene as six-membered ring without the hydrogen atoms, while other groups besides hydrogen must be written.

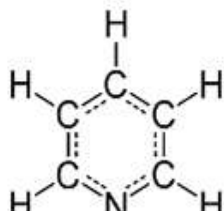
The carbon atoms of aromatic ring are bonded to each other by sigma bonds, and carbon atoms are also bonded to six hydrogen atoms by sigma bonds. Six electrons remain in the 2p<sub>z</sub> orbitals of carbon atoms of aromatic ring. These orbitals are perpendicular to plane of ring and parallel to each other. Therefore, they overlap laterally to form three  $\pi$  bonds. These bonds are non-local, which gives benzene its high stability.

Although benzene is aromatic, cyclic butadiene is non-aromatic because it has 4n delocalized  $\pi$  electrons, which doesn't yield whole number when Huckle rule is applied. However, the cyclic butadiene ion -2 is aromatic.

Non-aromatic molecules called aliphatic molecules. Aromatic molecules have better chemical stability that similar non-aromatic molecules. The rotation of  $\pi$  electrons in an aromatic molecule generates local magnetic field, which can be detected with nuclear magnetic resonance. Planar molecules with single ring contain 4n  $\pi$  electrons are called antiaromatic or Mobius (cyclooctatetraene COT) and are often unstable

### ***Pyridine***

Pyridine, abbreviated as (py), It is an organic compound. It has chemical formula C<sub>5</sub>H<sub>5</sub>N. that is heterocyclic aromatic compound. Pyridine structure consists of an unsaturated six-membered ring containing nitrogen atom. This ring is found in the structure of several important compounds, including azines and others such as niacin, pyroxine, isoniazid, and nicotine. It is used as solvent and as an intermediate in various reactions.



**Figure 4.** Pyridine.

### ***Furan***

Furan, also known as furfuran, is organic compound with formula C<sub>4</sub>H<sub>4</sub>O. It is heterocyclic aromatic compound, its structure consisting of unsaturated five-membered ring containing oxygen atom. It is aromatic, but not to the same degree as benzene, and is therefore more reactive. Tetrahydrofuran, from which it is derived, t is frequently used as a solvent and reactant, in addition to being chemical intermediate, that known to be carcinogenic substance. Furan is an aromatic compound with six  $\pi$  electrons: four in the two double bonds and the remaining two in the electron pair of the oxygen atom, thus fulfilling Hückel's rule.

Furan is prepared by treating corn or rice bran with hydrochloric acid (HCl) and heating it. This process removes water from the pentose sugar present in the bran, yielding furfural, which can then be converted to furan by removing the aldehyde group using high heat and a catalyst such as zinc oxide (ZnO).

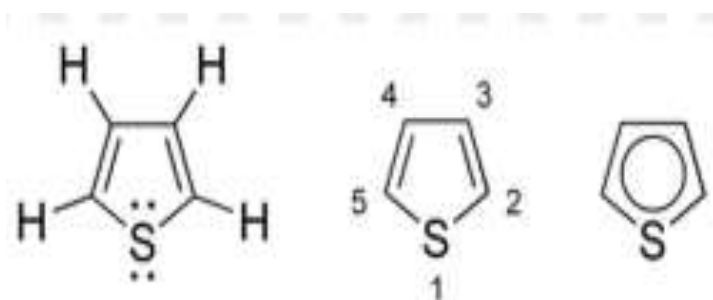


**Figure 5.** Furan.

### ***Thiophene***

Thiophene is cyclic organic compound, composed of an aromatic, unsaturated, 5-membered ring composed of (4) C. atoms and (1) sulfur atom, with the chemical formula  $C_4H_4S$ .

This compound is colorless liquid with benzene-like odor and exhibits aromatic properties similar to benzene. Thiophene and its derivatives are used in various fields, including the pharmaceutical industry as antibiotics, anti-inflammatories, and antifungals, the agricultural chemical industry, and in electrical conductors.



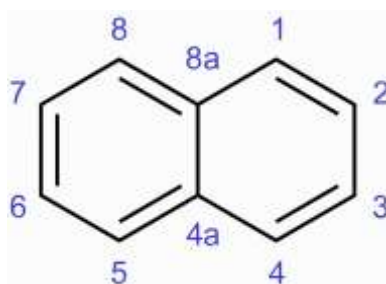
**Figure 6.** Thiophene.

### ***Polycyclic Aromatic Compounds***

Polycyclic aromatics are molecules composed of (2) or more simple aromatic rings bonded to each other with (2) adjacent C.atoms. adjacent carbon atoms and possessing stable system of delocalized  $\pi$  electrons, produced through incomplete combustion for organic materials. Some of these compounds are carcinogenic and hazardous to human health and the environment, entering the body through water, air, and food. Common examples include naphthalene, phenanthrene and anthracene.

## Naphthalene

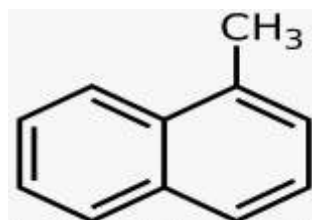
Naphthalene is type of polycyclic aromatic hydrocarbon (PAHs) because it contains two or more rings. N. is white crystalline solid aromatic hydrocarbon with formula  $C_{10}H_8$ , and simplest polycyclic aromatic hydrocarbon, where the molecule composed of (2) fused benzene rings. N. is volatile compound that is manufactured from coal tar and converted into phthalic anhydride for manufacture of plastics, dyes and solvents. In addition used as disinfectant and insecticide, especially in mothballs. It sublimates easily at room T. and is known to be the main component of mothballs used to protect clothes from moths.



**Figure 7.** Naphthalene

There are two methods for producing naphthalene:

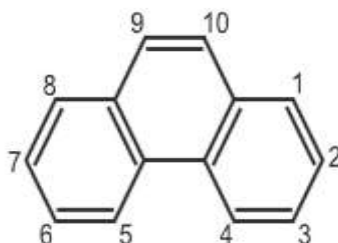
- 1) Production of N. from coal tar: Distillation and fractionation of coal tar, this method that most common of producing N., where the intermediate fraction (which contains most of the naphthalene) is crystallized after cooling, and the resulting crude N. can be refined by distillation, washing, and sublimation.
- 2) Production of naphthalene from oil: Since 1960, the extraction of N. from oil by alkylation of 1-methylnaphthalene, in hydrogen atmosphere in high T. and high pressure, has been commercial production process, followed by fractionation, decolorization, and purification by crystallization. The N. produced from petroleum is considered 99% pure.



**Figure 8.** 1-methylnaphthalene.

### *Phenanthrene*

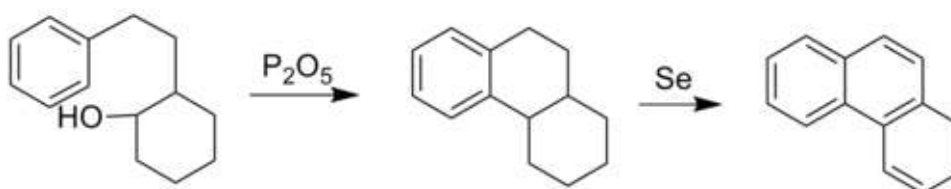
Phenanthrene is polycyclic aromatic hydrocarbon with three-membered hexagonal ring structure and the chemical formula  $C_{14}H_{10}$ , white crystalline powder, and does not mix with water, but is soluble in aromatic hydrocarbons as chloroform and ether. Ph. occurs naturally and is also synthesized.



**Figure 9.** Phenanthrene.

Ph. Using for production plastics, explosives, pharmaceuticals, pesticides, and dyes, in addition for production bile acids, steroids, and cholesterol. It is raw material for phenanthrexinone, which is widely used in the manufacture of dyes, agricultural chemicals, and preservatives.

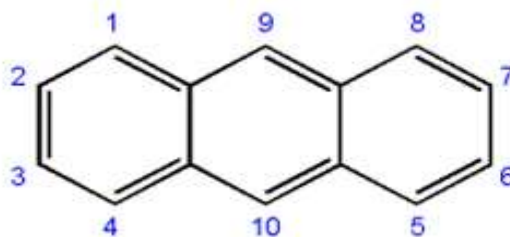
Ph. is prepared in the laboratory according to the Bardhan-Sengupta synthesis method, which involves an electron-loving aromatic substitution on cyclohexanol group linked by an alkyl bridge to benzene ring, using phosphorus pentoxide to close the ring; then by carrying out a dehydrogenation reaction using selenium metal.



**Figure 10.** Preparation of phenanthrene.

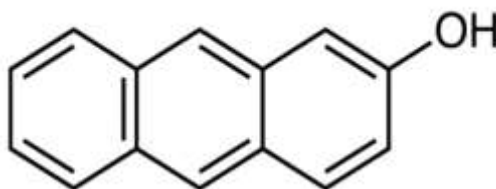
### *Anthracene*

Anthracene is chemical compound belonging to the (PAH) group, solid, in molecular formula  $C_{14}H_{10}$ . It consists of (3) benzene rings derived from tar. An. using for production of alizarin red dye, in Preserving wood, Pesticides, and packaging materials. It colorless compound but gives a blue color (peak at 400-500 nanometers) fluorescence under ultraviolet light.



**Figure 11.** Anthracene.

Anthracene derivatives with hydroxyl group include 1-hydroxy anthracene and 2-hydroxyanthracene  $C_{14}H_{10}O$ , analogous to phenol and naphthol, as well as hydroxyanthracene (also called anthrole) and anthracnol. Hydroxyanthracene derivatives are pharmacologically active.



**Figure 12.** 1-hydroxyanthracene.

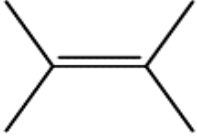
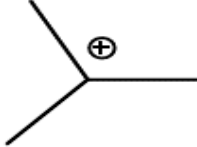
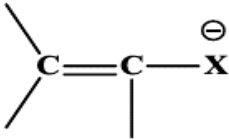
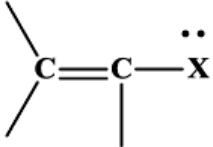
Anthracene can be prepared from coal tar by boiling it, removing the oil fraction, and then subliming it to remove impurities. Alternatively, via the Friedel-Crafts reaction, using benzyl chloride, or the Haworth method of synthesis, phthalic anhydride is treated in benzene solution with aluminum chloride to produce benzoylbenzoic acid.

### 3. HÜCKEL'S LAW FOR CALCULATING AROMATICITY

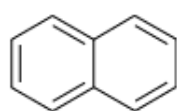
For compound to be aromatic, the following conditions must be met:

- 1) It must be cyclic.
  - 2) It must be planar (all atoms in the ring must be  $sp^2$  hybridized): meaning each atom in the ring has  $p_z$  orbital.
  - 3) The  $\pi$  bonds must be in an alternating state.
  - 4) The number of  $\pi$  electrons must be  $n + 2$ .
- $n = 0, 1, 2, 3 \dots$  and  $n$  represents the number of rings.

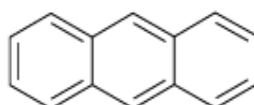
**Table 1.** SP<sup>2</sup> hybridized atoms.

SP <sup>2</sup> hybridized atoms	Example	Number of $\pi$ electrons
Atoms that are bonded by double bond		2 electrons per double bond, and each atom contributes one electron
Carbon atoms that carry positive charge		Zero electrons on an atom that carries positive charge
Atoms carrying negative charge have double bond nearby		2 electrons on the atom that carries negative charge
Atoms that carry free pair of electrons nearby double bond		2 electrons on an atom that carries free electron pair

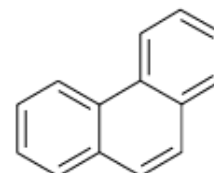
Examples of aromatic and non-aromatic compounds:



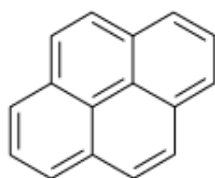
naphthalene



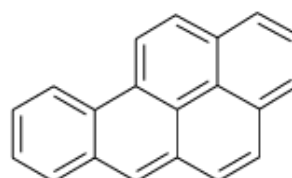
anthracene

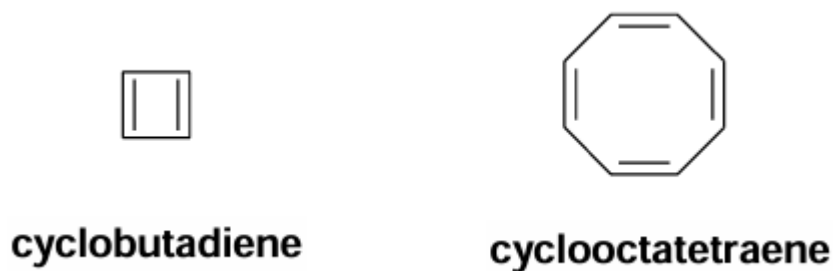


Phenanthrene



Pyrene

benzo[a]pyrene  
carcinogenic compound resulting  
from burning cigarettes**Figure 13.** aromatic compounds.



**Figure 14.** non-aromatic compounds.

#### **4. TYPES OF POLLUTION FROM POLYCYCLIC AROMATIC HYDROCARBONS**

The problem of environmental pollution, its types, causes, and methods of treatment, is currently a top priority for both major industrialized and developing nations worldwide, given the direct threat it poses to human health and other living organisms.

There are more than one hundred hazardous (PAHs) that impact on environment and human health through water use, inhalation of air, or indirectly through the consumption of food and animal products.

##### **Impact on The Environment**

Aromatic compounds negatively impact the environment by polluting air, water, and soil, posing serious threat to living organisms and ecosystems. Most polycyclic aromatic hydrocarbons cannot dissolve in water, that reduces its ability to move in aquatic environment. Bicyclic *PAHs* and the lesser tricyclic *PAHs* are dissolve in water, make it more accessible for biosynthesis. Bicyclic *PAHs* are sufficiently volatile to tetracyclic *PAHs* stand out in Atmosphere, mostly in form gases, although physical state for tetracyclic aromatic polycyclic hydrocarbons can depend on T. Conversely, compounds containing (5) or more rings have low solubility in water and low volatility, and so mostly for solid state, attached to air pollution particles, soil, or sediments. For the solid state, compounds less biosynthetic, which increases their stability in the environment.

Aromatic compounds such as *PAHs* and volatile organic compounds (VOCs) are major air pollutants, produced due to engine exhaust and tobacco, waste incinerators, in grilled meats and grains, or when biomass burns at low T. as in forest fires.

U.S. Environmental Protection Agency (EPA) has selected fourteen hazardous compounds from the *PAHs* family to monitor their concentration limits due to their greater prevalence and presence in the environment.

**Table 2.** Carcinogenic Activity of Polycyclic Aromatic Hydrocarbons.

Compound	Molecular Weight (g/mol)	Melting Point (°C)	Boiling Point (°C)	Aqueous Solubility (µg/L at 25°C)	Carcinogenic Activity
Naphthalene	128.00	81	200	31,700	0
Fluorene	166.22	115	298	1,980	0
Chrysene	228.29	254	448	2	+
Acenaphthene	154.21	96.2	279	3,930	0
Benzo(a)anthracene	228.30	158.4	400	14	+
Fluoranthene	202.26	107	384	260	0
Benzo(k)fluoranthene	252.32	217	480	–	++
Indeno(1,2,3-cd)pyrene	276.00	161–163.5	–	–	+
Phenanthrene	178.23	99–101	340	1,290	0
Pyrene	202.26	156	393	135	0
Benzo(a)pyrene	252.30	179	495	3,800	++
Acenaphthylene	152.21	92	265–275	16,100	0
Anthracene	178.23	216.4	340	73	0
Benzo(b)fluoranthene	252.32	168	–	–	++

(0) Non-carcinogenic, (+) Carcinogenic up to 33%, (++) Carcinogenic more than 33%

### Impact on Human Health

The impact on humans varies worldwide, depending on reasons as the amount of smoke and types of fuel (including those used for cooking), pollution from power plants and industrial facilities, and emissions from gasoline, diesel, and electric vehicles, as well as coal and fuel oil refineries. Burning solid fuels like coal and biofuels in homes for cooking and heating is dominant global source of PAH emissions, leading to high percentage of air polluted with particles inside the home, especially for women and kids that spend more time indoors.

Polycyclic aromatic hydrocarbons (PAHs) are considered dangerous pollutants, as some have toxic effects and others are carcinogenic to humans. These pollutants are released into the air through dry or wet precipitation by rain, thus transferring the pollution problem from the air to water bodies and soil, especially in urban and industrial areas, as well as areas adjacent to and far from the sources of these pollutant emissions, such as agricultural areas.

A report from Centers for Disease Control and Prevention (CDC) indicated to polycyclic aromatic hydrocarbons (PAHs) may be cause cancer, and some people that inhaled or in contact with mixture of polycyclic aromatic hydrocarbons or other chemicals for extended periods have diagnosed cancer. Some PAHs caused cancer in laboratory animals when inhaled air containing them (lung cancer), ingested food (stomach cancer), or used as skin ointment (skin cancer).

The CDC also conducted several experiments to investigate how PAHs are converted in the body into chemicals that can bind to substances within the body.

### Methods of Infection

- 1) Inhalation of air containing polycyclic aromatic hydrocarbons (PAHs) in workplaces where coke and coal tar are manufactured, asphalt plants, smoked fish processing plants, and municipal waste incineration facilities.
- 2) Inhalation of air containing PAHs from cigarette smoke, wood smoke, vehicle exhaust, asphalt roads, or smoke from burning agricultural residues.
- 3) Consumption of roasted or overcooked meat, grains, flour, bread, vegetables, fruits, or meats contaminated with acid solutions.
- 4) Ingestion of polluted water or cow's milk.
- 5) Exposure of infants to PAHs born to mothers living near hazardous waste sites through breast milk.

## 5. CONCLUSION

The research yielded several findings, which present as follows:

- 1) Aromatic compounds are unsaturated organic hydrocarbon compounds that share the characteristic of containing benzene ring. All these aromatic compounds share specific properties that distinguish them from aliphatic compounds.
- 2) Benzene is the simplest aromatic compound.
- 3) There are more than one hundred hazardous *PAHs* that impact human health through inhalation of water or air, or indirectly through the use of food and animal products.
- 4) Most polycyclic aromatic hydrocarbons are insoluble in water, that reduces its solubility and movement in aquatic environments.
- 5) Contributing factors to this pollution include smoking, various fuels (including those used for cooking), pollution from power plants and industrial facilities, and emissions from vehicles powered by gasoline, kerosene, electricity, and even coal or fuel oil refineries.
- 6) Burning solid fuels is considered such as coal in houses for cooking and heating is major global source of of polycyclic aromatic hydrocarbon emissions.

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