

## Quadrant II – Transcript and Related Materials

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### Notes

Simple aromatic rings, also known as simple arenes or simple aromatics, are aromatic organic compounds that consist only of a conjugated planar ring system. They are usually found as substructures of more complex molecules ("substituted aromatics").

#### What are Aromatic Compounds

Aromatic compounds, originally named because of their fragrant properties, are unsaturated hydrocarbon ring structures **which have one or more planar six-carbon rings called benzene rings, to which hydrogen atoms are attached with the general formula  $C_nH_n$**  that exhibit special properties, including unusual stability, due to their aromaticity.

#### Physical Properties of Aromatic Hydrocarbons

Some general properties of aromatic hydrocarbons have been listed below.

1. Aromatic compounds are generally nonpolar and immiscible with water
2. As they are often unreactive, they are useful as solvents for other nonpolar compounds.
3. These compounds exhibit *aromaticity* (additional stability granted by resonance)
4. Due to their high ratio of carbon to hydrogen, aromatic compounds are characterized by a strong and sooty yellow flame which is yellow in colour.
5. These compounds generally *undergo electrophilic substitutions and nucleophilic aromatic substitution reactions*.
6. It can be noted that these compounds can be either monocyclic or polycyclic.

**The first compound that was categorized as an aromatic hydrocarbon was benzene** is the simplest aromatic hydrocarbon (or arene).

1. Benzene is the parent compound and its substituent is prefixed to Benzene.

2. Aromatic compounds are named based on the number and type of substituents on the ring.

When there is a single substituent on a benzene ring and the substituent contains six or fewer carbons, the substituent is included as a prefix to benzene.

If the Aromatic Compound is with a Single Substituent it is called as Monosubstituted benzene.

Benzene whose only one hydrogen atom is replaced by alkyl/functional group

For eg. Chlorobenzene, Nitrobenzene and Bromobenzene

If Alkyl groups are added for eg

- methyl (for a single carbon) – Methylbenzene (Toluene)
- ethyl (for two carbons) – Ethylbenzene
- propyl (for three carbons) – Propylbenzene

If the substituent contains more than six carbons, an aromatic ring bonded to an 8-carbon chain would be 1-phenyloctane.

Another example of substituted aromatic compounds is when Alkyl group is linked to functional group **Benzyl alcohol**

Many monosubstituted benzenes have common names and are known by their common names Phenol, Toluene, Aniline, Benzoic acid, Anisole

When the aromatic compounds are with multiple substituents, ring atoms are numbered to minimize the numbers assigned to the substituted positions are called as Disubstituted benzene. Benzene whose two hydrogen atoms are replaced by alkyl/functional group.

There are three different ways that two groups can be attached to a benzene ring, so a prefix—ortho, meta, or para—can be used to designate the relative position of the two substituents.

1,2-dibromobenzene , 1,3- dibromobenzene and 1,4-dibromobenzene

### **PAH**

Polyaromatic hydrocarbons commonly referred to as PAHs also known as Polycyclic aromatic hydrocarbons or polynuclear aromatic hydrocarbons are a large group of organic compounds containing only carbon and hydrogen—that are composed of two or more fused aromatic rings

Polycyclic aromatic hydrocarbons (PAHs) are a group of approximately 10, 000 compounds that are atmospheric, water, and soil pollutants.

#### **Characteristics**

1. The structure of a PAH consists of molecules containing two or more fused six-carbon atom aromatic rings; only hydrogen and carbon are present in the molecules.
2. PAHs are uncharged, non-polar molecules have a relatively low solubility in water, but are highly lipophilic

3. The higher the number of benzene-rings the PAH has, the higher the molecular weight, but the lower the solubility in water.
4. In the atmosphere, PAHs can react with pollutants such as ozone, nitrogen oxides and sulfur dioxide, yielding diones, nitro- and dinitro-PAHs, and sulfonic acids, respectively.

Some of the examples of PAH's are given

The simplest is Benzene from which the other PAH's are derived

**Naphthalene**, Anthracene, Phenanthrene, Pyrene, Benzo[e]-pyrene, Coronene, Triphenylene

One simplest common example of these polycyclic hydrocarbons is naphthalene, having two aromatic rings. Naphthalene is an important item in the production of mothballs. Naphthalene, the two-benzene-ring PAH, often present in significant amounts in petroleum, is relatively volatile, soluble, and degradable.

Comparatively higher molecular weight species such as phenanthrene (three-benzene-ring PAH (Phe)).

It is used in the synthesis of drugs, dyes and explosives.

Pyrene (Pyr) is having four benzene rings formed during incomplete combustion of organic compounds and is commercially used to make dyes and dye precursors.

Benzo[e]pyrene is a (five-benzene-ring PAH (BeP)) can be found in weathered crude oils reaching coastal wetlands and found in cigarette smoke and produced by the incomplete oxidation of organic compounds in tobacco. When ingested/inhaled are oxidized to carcinogenic products.

### **Sources of PAHs**

Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous, persistent environmental organic contaminants generated by natural **or manmade or thermal incomplete** combustion of a variety of organic compounds.

High-temperature cooking, such as grilling, smoked fish, burnt toast will form PAHs in meat and other foods.

PAHs are released from burning coal, oil, tar deposits, crude oil, gasoline, trash, tobacco, wood, tobacco, cigarette smoke or when biomass burns in forest fires.

The dominant sources are thus from human activity: wood-burning and combustion of other biofuels such as dung or crop residues. Emissions from vehicles such as cars and trucks can be a substantial outdoor source of PAHs in particulate air pollution

### **Effects**

Released into the environment they tend to remain in surface soils and do not migrate in groundwaters except Naphthalene.

These compounds are said to be pollutants and may also be degraded by some microorganisms in the soil.

The higher ringed PAHs are quite resistant to biodegradation due to their complexity and very low solubility.

PAHs are considered hazardous because of cytotoxic, mutagenic, and carcinogenic effects. Cancer is a primary human health risk of exposure to PAHs.

Exposure to PAHs has also been linked with cardiovascular disease and poor fetal development.