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Aromatic compounds and their applications in dentistry

Aromatic compounds: -

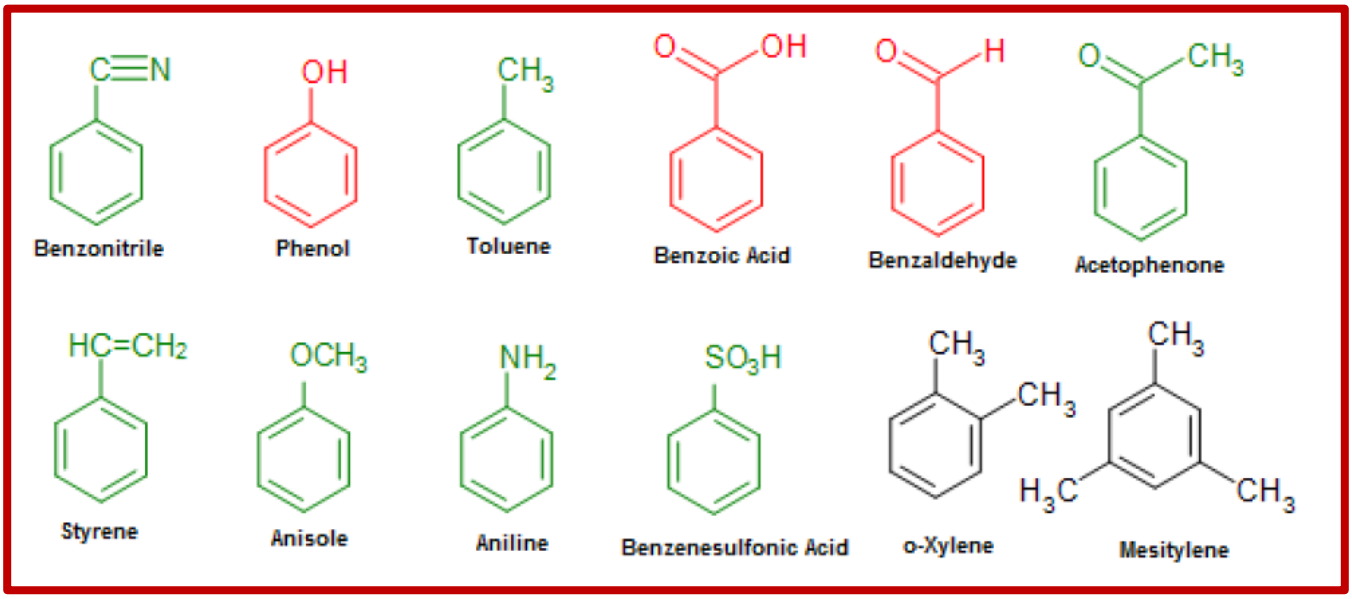
Aromatic compounds are chemical compounds that consist of conjugated planar ring systems accompanied by delocalized pi-electron clouds in place of individual alternating double and single bonds.

They are also called aromatics or arenes. The best examples are toluene and benzene. Aromatics require satisfying Huckel's rule. Plants and micro-organisms have an exclusive route to benzene-ring compounds. The great majority of aromatic compounds in nature, therefore, are produced by plants and micro-organisms, and animals are dependant upon plants for many aromatic compounds either directly or indirectly.

On the other hand, aromatic compounds are a large family of compounds comprised of a six-membered ring or more complex structure. Notably, aromatic compounds are not limited to hydrocarbons as there are aromatic compounds like thiophene and pyridine which have S and N in their structure.

Aromatic Compounds Examples

Aromatic hydrocarbon, are hydrocarbons containing sigma bonds and delocalized pi electrons between carbon atoms in a ring. For example, benzene. They are known as aromatic due to their pleasant smell.

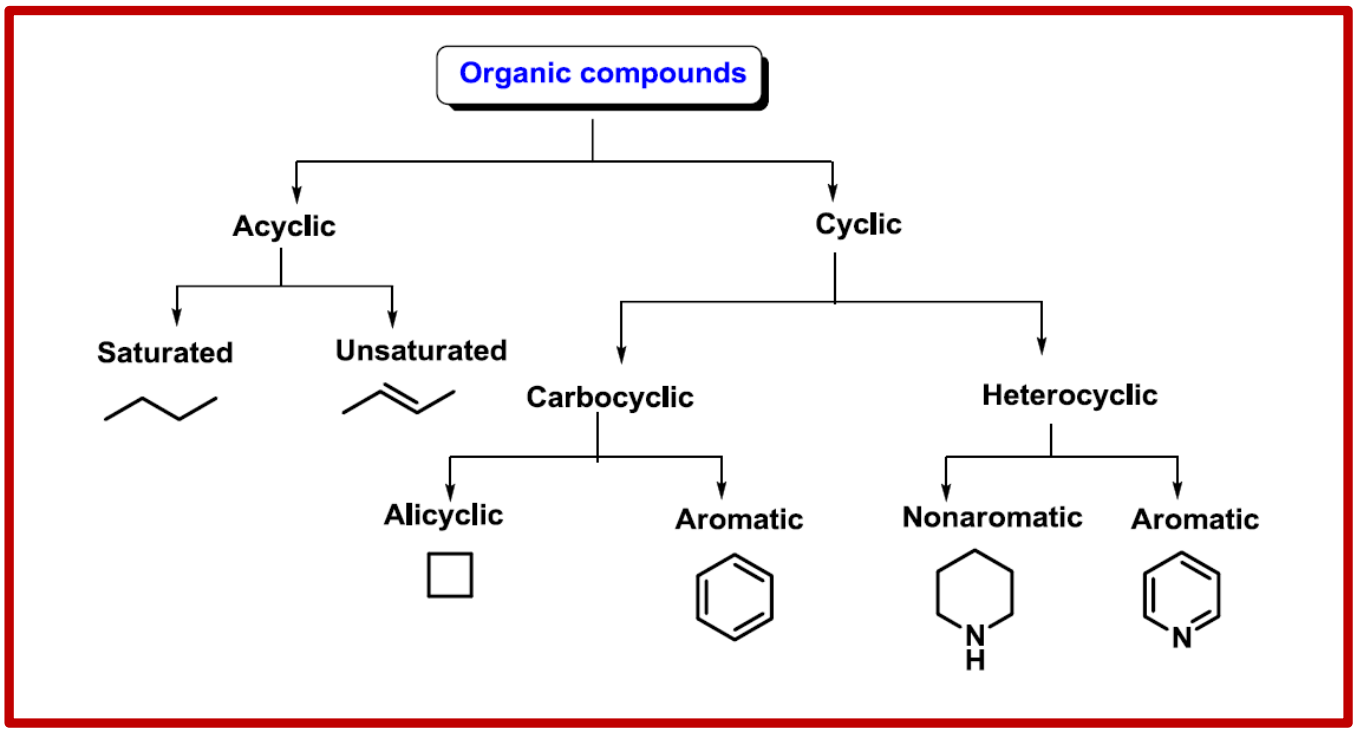


Compounds are classified as aromatic if they are able to exhibit the following properties:

1) The molecule is cyclic and contains conjugated high or low electron density areas.
2) The molecule is very stable compared to their aliphatic counterparts.
3) The molecule is planar to allow easier delocalization of the π electrons.
4) All atoms in the cycle contain a p-orbital for overlap.
5) The molecule follows the Huckel 4n + 2 π electron rule where n should be an integer.
6) The compound is considered to be aromatic if it is able to exhibit all of the properties Included in the chart below.
7) Otherwise, the compound can be classified as either a non-aromatic or anti-aromatic compound.

An aromatic compound is considered a big family of compounds as it comprises of compounds with a sixmembered ring, to more complex structures. Aromatic compounds are also not limited to hydrocarbons as there are also aromatic compounds like thiophene and pyridine that are considered aromatic, even if they have S and N in their structure. Ions can also be considered as aromatic.

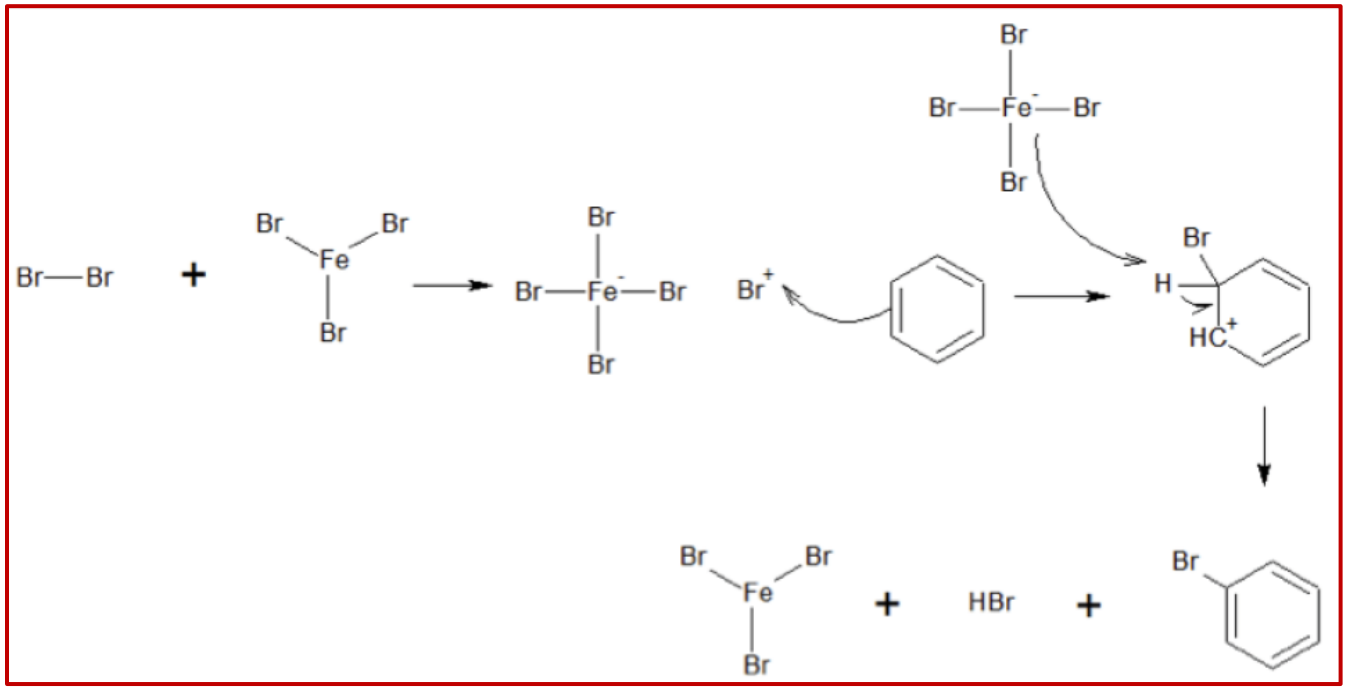
According to the character of chain of carbon atoms:

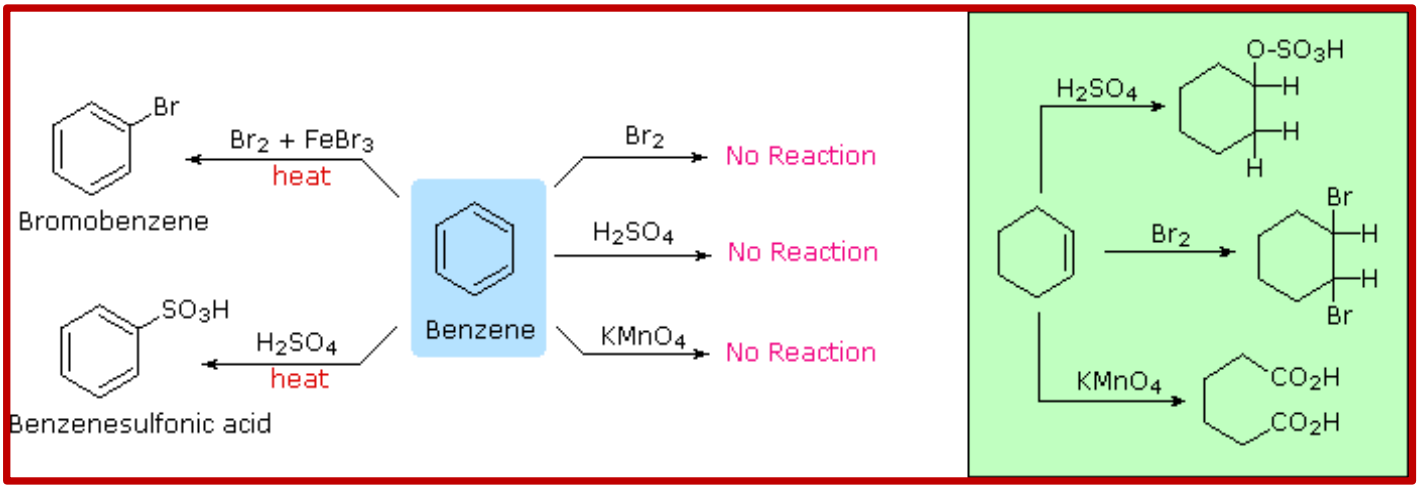


Halogenation:- Bromination reaction of benzene

Aromatic compounds, unlike ordinary alkenes, are less reactive compared to their acyclic counterparts due to their relative stability afforded by π electron delocalization. In a halogenation reaction known as bromination, Br_2 can readily react with ethane to produce dibromoethane. This is not true for benzene. For the bromination reaction to proceed in benzene, a catalyst such as $FeBr_3$ is needed which provides a different mechanism for the reaction to proceed.

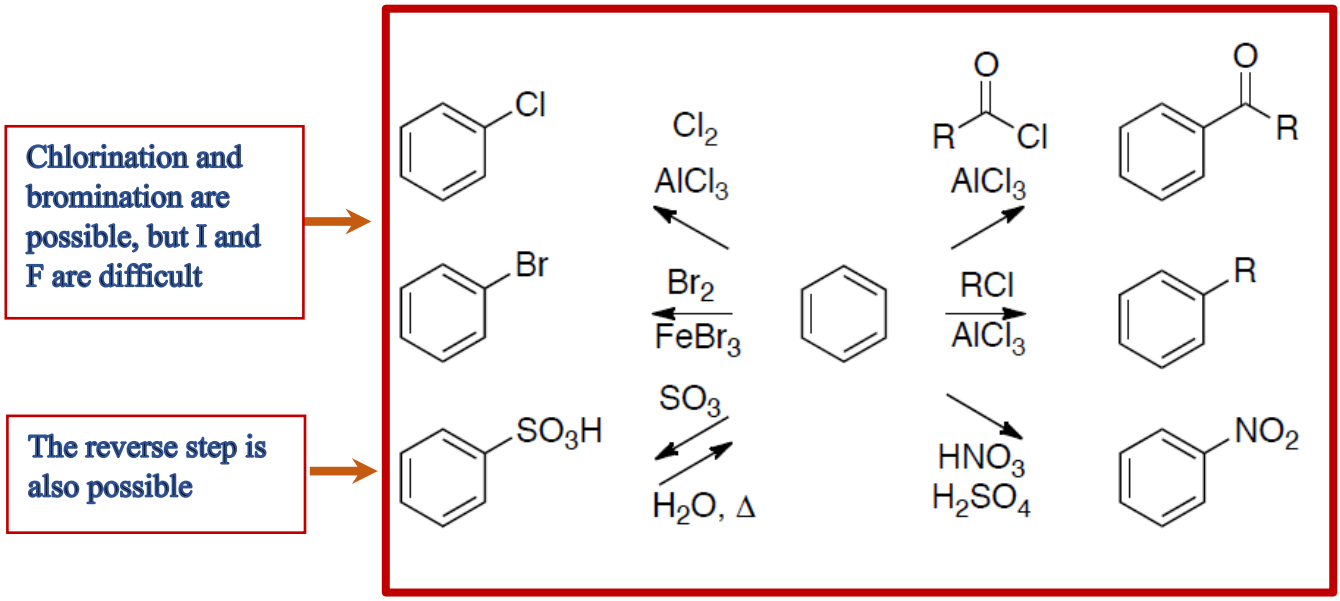
The 1st step in the reaction is the polarization of the Br_2 molecule by $FeBr_3$. In the process, a more electrophilic molecule is produced in the form of $FeBr_4– Br+$. The presence of Br^+ makes $FeBr_4– Br^+$ more electrophilic than an ordinary Br_2 molecule. The $FeBr_4– Br^+$ will then attack the benzene molecule and a base will remove the proton in the process. Below is the mechanism of the reaction.





where an aromatic ring can have different substituents added

While this allows a variety of substituents, the range is far less than a chemist would ultimately desire.



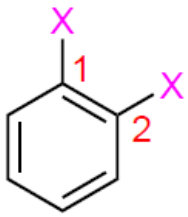
Nomenclature of Disubstituted Benzenes

With disubstituted benzenes there are three distinct positional isomers which can occur and must be identified in thecompounds name. Although numbering can be used to indicate the position of the two subsituents it is much morecommon for the compounds to be named using prefixes. These prefixes are italicized and are often abbreviated with asingle letter. They are defined as the following:

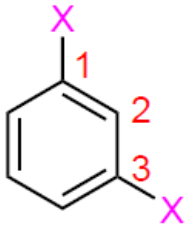
ortho- (o-): 1,2- (next to each other in a benzene ring)

meta- (m): 1,3- (separated by one carbon in a benzene ring)

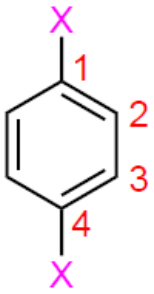
para- (p): 1,4- (across from each other in a benzene ring)



***ortho*-Disubstituted**
(1,2)



***meta*-Disubstituted**
(1,3)

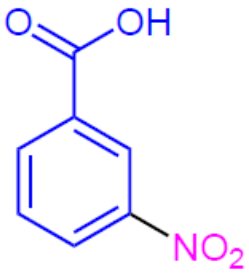


para-Disubstituted
(1,4)

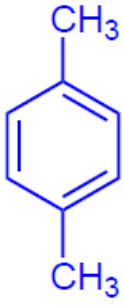
If any do appear then the compound is not named as a benzene but with a different parent name. Thesecompounds are named as such:

Position prefix - Name of the substituent + Name of parent chain.

ortho-Chlorophenol



meta-Nitrobenzoic acid

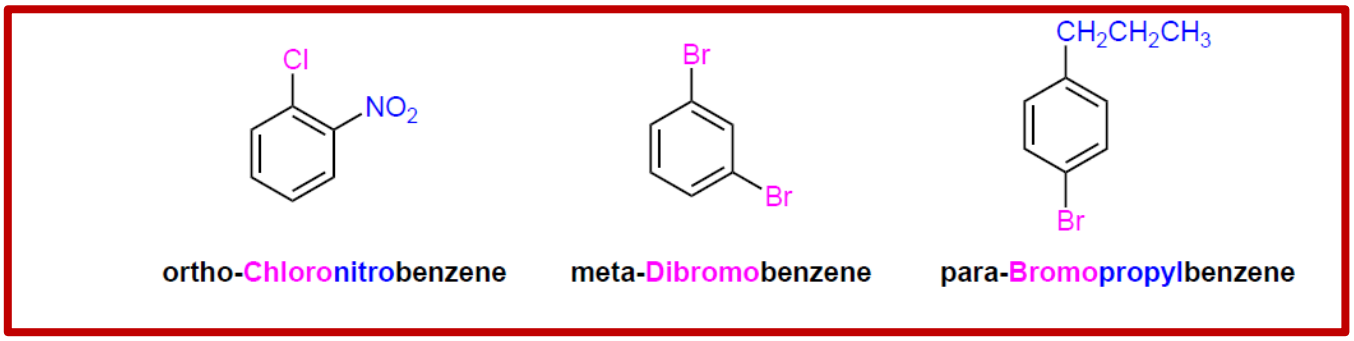


para-Xylene

The compound is named as such: Position prefix -

Names of the substituents in alphabetical order + benzene.

Remember if two of the same substituents appears then the prefix di- is used before the substituent's name.

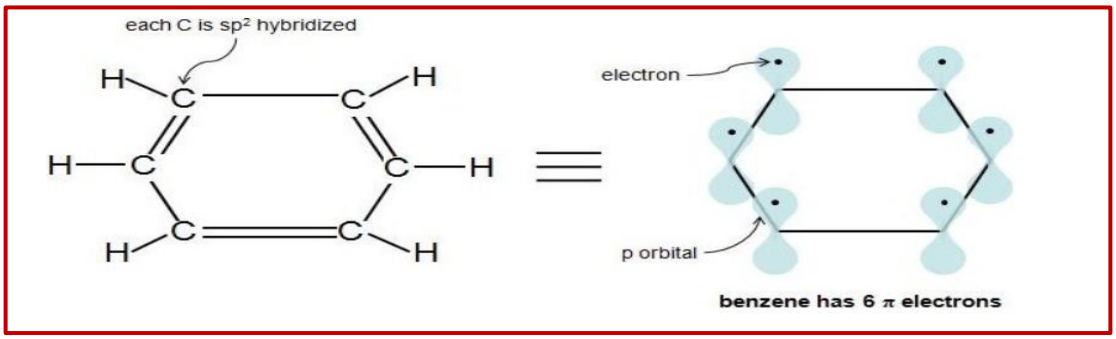


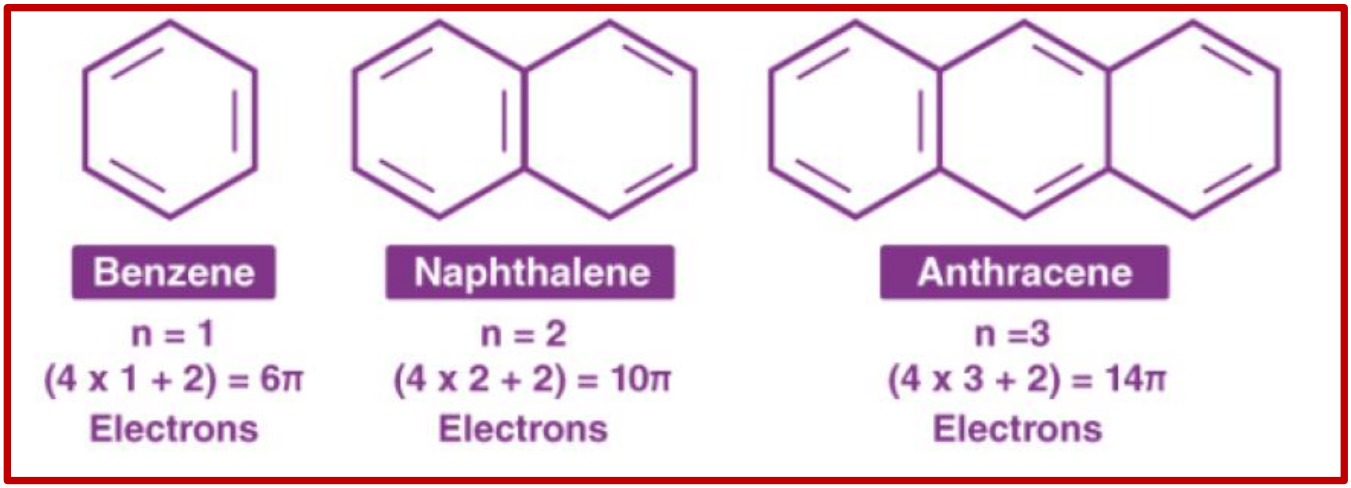
Huckel's Rule of Aromaticity

Huckel's rule states that only planar, fully conjugated monocyclic polyenes having 4n + 2 π electrons, where n is an integer, that is, n = 0,1, 2, 3, 4, etc., should possess aromatic stability. An aromatic compound must be planar and contain a cyclic cloud of π electrons below and above the plane of the molecule. It contains SP hybridized carbon atoms and must obey the Huckel rule.

According to this rule, the ring system must have (4n+2) π electrons, where n is any whole number (0, 1, 2, 3, etc). On this basis the ring systems which have 2(n=0), 6(n=1), 10(n=2), 14(n=3) etc pi electrons are aromatic.

Typical examples of aromatic compounds are benzene, naphthalene, and anthracene.





HETEROCYCLIC COMPOUNDS

Heterocyclic compound is the class of cyclic organic compounds those having at least one hetero atom (i.e. atom other than carbon) in the cyclic ring system. The most common heteroatoms are nitrogen (N), oxygen (O) and sulphur (S).

Heterocyclic compounds are frequently abundant in plants and animal products; and they are one of the important constituent of almost one half of the natural organic compounds known. Alkaloids, natural dyes, drugs, proteins, enzymes etc. are the some important class of natural heterocyclic compounds.

Heterocyclic compounds can be easily classified based on their electronic structure. Heterocyclic compounds are primarily classified as saturated and unsaturated.

The saturated heterocyclic compounds behave like the acyclic derivatives with modified steric properties. Piperidine and tetrehydrofuran are the conventional amines and ethers of this category. However, unsaturated heterocyclic compounds of 5- and 6- member rings have been studied extensively because of their unstrained nature.

The unstrained unsaturated heterocyclic compounds include Pyridine, Thiophene, Pyrrole, Furan and their benzo fused derivatives. Quinoline, Isoquinoline, Indole, Benzothiophene, and Benzofuran are some important example of benzo fused heterocycles. Heterocyclic compounds have a wide application in pharmaceuticals,

agrochemicals and veterinary products and dentistry through salivary secretions, which contains amylase.

Moreover, many heterocyclic compounds are very useful and essential for human life. Various compounds such as hormones, alkaloids antibiotic, essential amino acids, hemoglobin, vitamins, dyestuffs and pigments have heterocyclic structure.

heterocyclic compounds, such as Pyrrole, Furan, Thiophene, Pyridine and Piperidine etc.

CLASSIFICATION OF HETEROCYCLIC COMPOUNDS

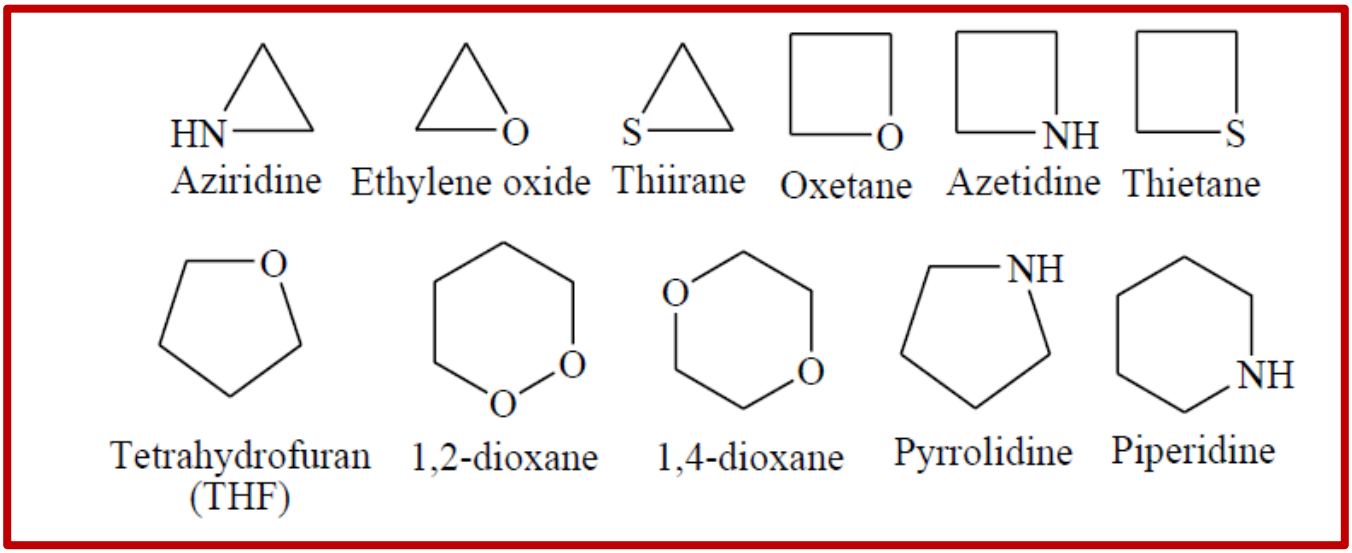
Based on the structural and electronic arrangement the heterocyclic compounds may be classified into two categories.

i. Aliphatic heterocyclic compounds

ii. Aromatic heterocyclic compounds

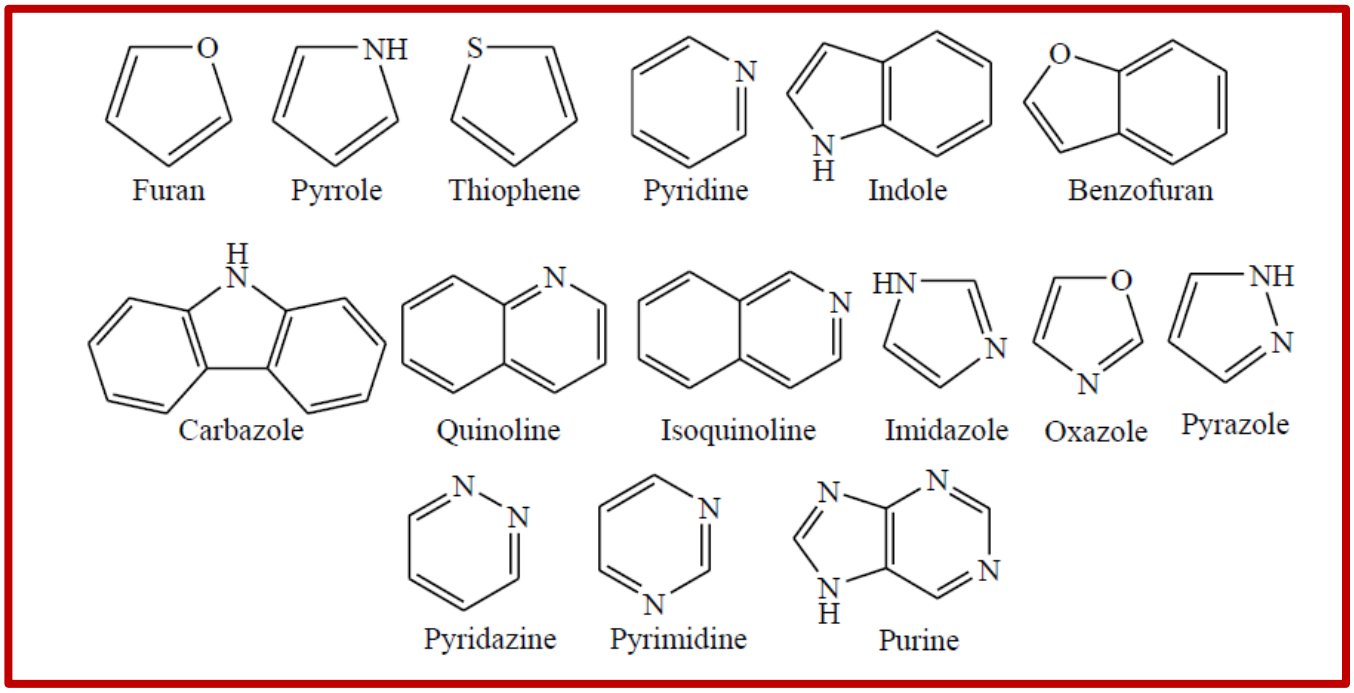
The aliphatic heterocyclic compounds are the cyclic amines, cyclic amides, cyclic ethers and cyclic thioethers. Aliphatic heterocycles those do not contain double bonds are called saturated heterocycles. The properties of aliphatic heterocycles are mainly affected by the ring strain.

Examples of aliphatic heterocyclic compounds are shown.



Examples of aliphatic heterocyclic compounds

However, aromatic heterocyclic compounds are analogous of benzene. The aromatic heterocyclic compounds also follow the Huckel's rule. According to Huckel's rule an aromatic compounds must be cyclic in nature with planar geometry due to conjugate double bonds and must have (4n+2)π electrons. Examples of aromatic heterocyclic compounds.



Examples of aromatic heterocyclic compounds

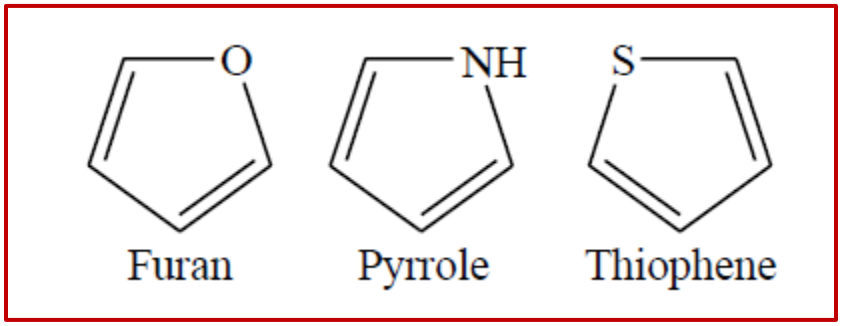
A hetero cyclic ring may comprise of three or more than three atoms, which may be saturated or unsaturated. Also, heterocyclic ring may contain more than one heteroatom which may be either similar or different.

Based on the variety of structure, the heterocyclic compounds may also be divided in to three categories.

1. Five membered heterocyclic compounds: These heterocyclic compounds may be considered to be derived from benzene by replacing one C=C bond by a hetero atom with a lone pair of electrons.

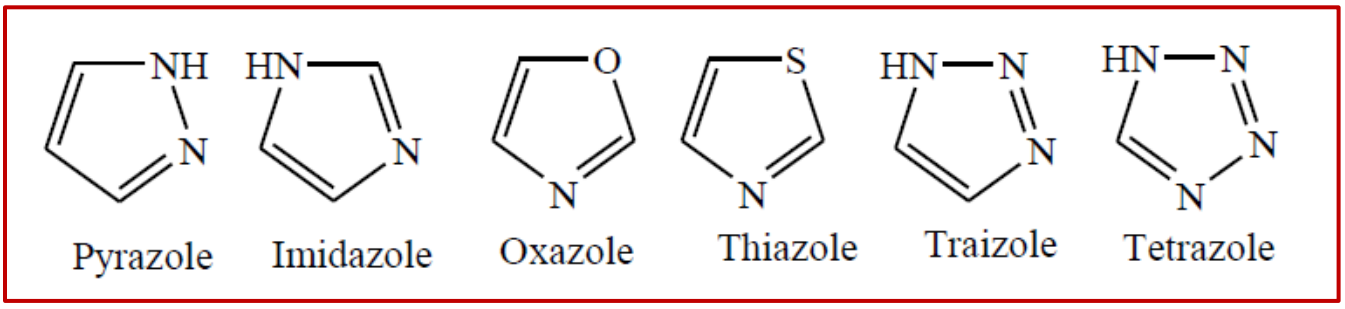
Based on number of hetero atom present in the cyclic ring this class of heterocyclic compounds may be further subdivided in to following categories.

a). Heterocyclic compounds with one hetero atom: Common examples of this class of compounds are furan, thiophene and pyrrole.



Five member heterocyclic compounds with one hetero atom

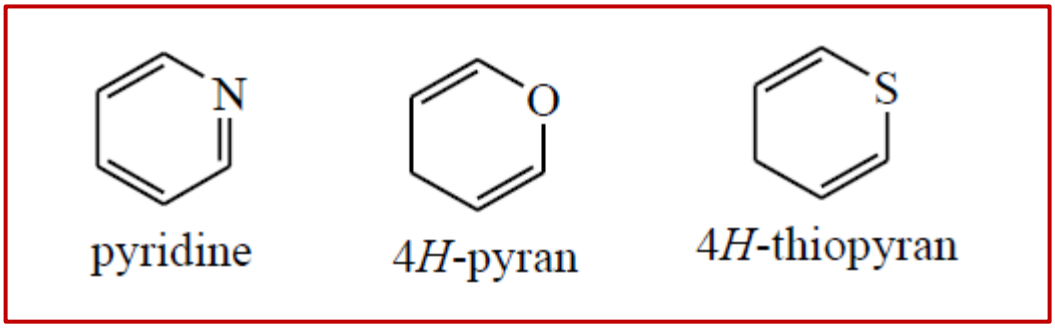
b). Heterocyclic compounds with more than one hetero atom: These hetero atoms may be same or different. Common examples of this category of heterocyclic compounds are pyrazole, imidazole, thiazole, oxazole, triazole and tetrazole etc.



Five member heterocyclic compounds with two hetero atom

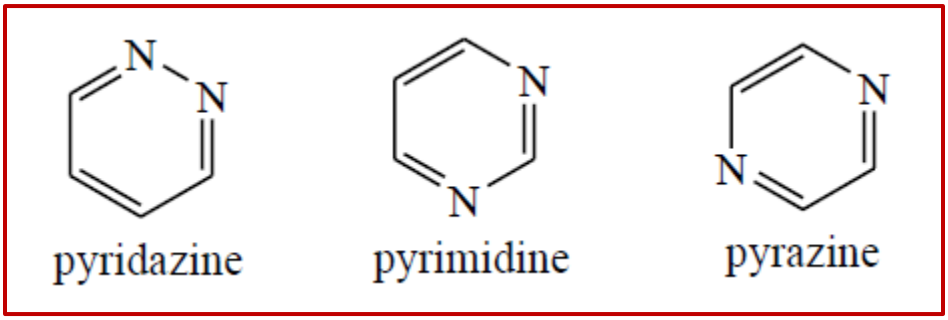
2. Six membered heterocyclic compounds: This class of compounds may be considered to be derived from the replacement of a carbon atom of benzene by an iso-electronic atom. Similar to the five membered heterocyclic compounds, the six membered heterocyclic compounds may also be subdivided in to following categories.

a). Heterocyclic compounds with one hetero atom: Common examples of this class of compounds are pyridine, pyran, thiopyran etc.



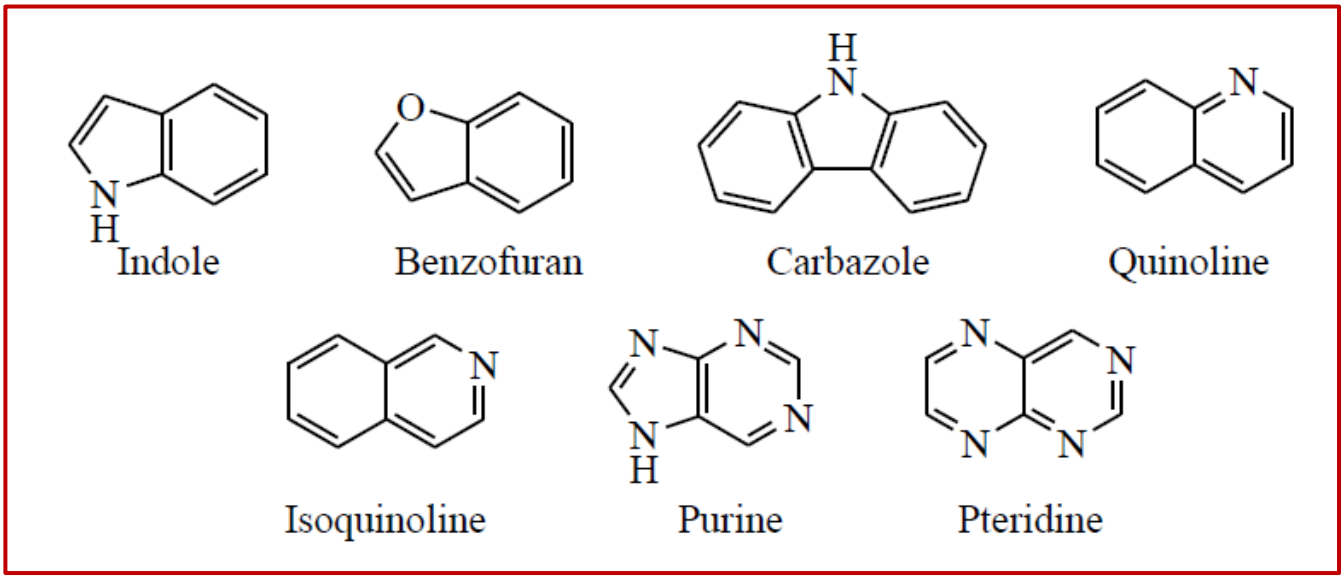
Six member heterocyclic compounds with one hetero atom

b). Heterocyclic compounds with more than one hetero atom: Common examples of this class of compounds are pyridazine, pyrimidine, pyrazine etc.



Six member heterocyclic compounds with more than one hetero atom

3. Fused or condensed heterocyclic compounds: This class of compound may consist two or more fused rings which may be partly carbocyclic and partly heterocyclic, common examples of this category of heterocyclic compounds are Indole, Quinoine, Isoquionoline, Cabazole etc; or may be completely heterocyclic, common examples of this category of heterocyclic compounds are purine, pteridine etc.



Fused or condensed heterocyclic compounds

Frequently Asked Questions – FAQs

What is an aromatic organic compound?

Aromaticity is a property in organic chemistry of cyclic (chain-shaped), planar (flat) structures with a ring of resonance bonds that gives greater stability compared to other geometric or connective arrangements with the same collection of atoms.

What are heterocyclic aromatic compounds?

A heterocyclic compound is an organic compound where an atom other than carbon has substituted one or more of the carbon atoms in the molecule's backbone. Nitrogen, oxygen, and sulphur are normal hetero atoms.

What is the general formula of aromatic compounds?

Aromatic hydrocarbons are compounds that contain benzene as part of their structure, also known as aromatic compounds. Benzene, with formula C6H6, is a cyclic hydrocarbon.

What is the difference between aliphatic and aromatic?

The carbon compounds are related in a straight chain way in aliphatic compounds. In aromatic compounds, the carbon compounds are associated with conjugated pi electrons in the manner of a ring structure.

Are all aromatic compounds cyclic?

Cyclic compounds may or may not be aromatic; benzene is an example of a cyclic aromatic compound, while cyclohexane is non- aromatic. Organic compounds that are not aromatic are known as aliphatic compounds, but only aromatic rings are especially stable.

What do you understand by heterocyclic compounds?

Heterocyclic compound is the class of cyclic organic compounds those having at least one hetero atom (i.e. atom other than carbon) in the cyclic ring system. The most common heteroatoms are nitrogen (N), oxygen (O) and sulphur (S). Heterocyclic compounds are frequently abundant in plants and animal products; and they are one of the important constituent of almost one half of the natural organic compounds known. Alkaloids, natural dyes, drugs, proteins, enzymes etc. are the some important class of natural heterocyclic compounds. Heterocyclic compounds have a wide application in pharmaceuticals, agrochemicals and veterinary products. Many heterocyclic compounds are very useful and essential for human life. Various compounds such as hormones, alkaloids antibiotic, essential amino acids, hemoglobin, vitamins, dyestuffs and pigments have heterocyclic structure.