

Organic Chemistry

2nd stage

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Lecture 1: Aromatic compound

Department of Bio chemistry

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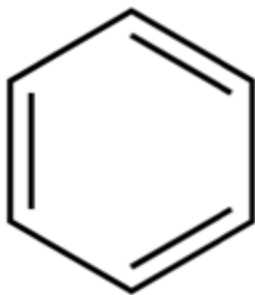
1.1 Aromatic compound

Aromatic compounds are unusually stable and have important chemical and synthetic uses. But, what makes a compound aromatic? A short list of rules, discovered by Eric Huckel in the 1930's, lists the properties of aromatic compounds.

The Huckel aromaticity rules are:

1. Molecule is cyclic
2. Have one p orbital per atom of the ring (conjugated)
3. Be planar, in an sp^2 hybridized orbital, over every atom of the ring
4. Have a closed loop of $4n+2$ pi-bond electrons, where n is equal to any integer (0,1,2,3,...)

Benzene



Since benzene has 6 pi electrons:

$$4n + 2 = 6$$

Find n:

$$4n + 2 = 6$$

$$4n = 6 - 2$$

$$4n = 4$$

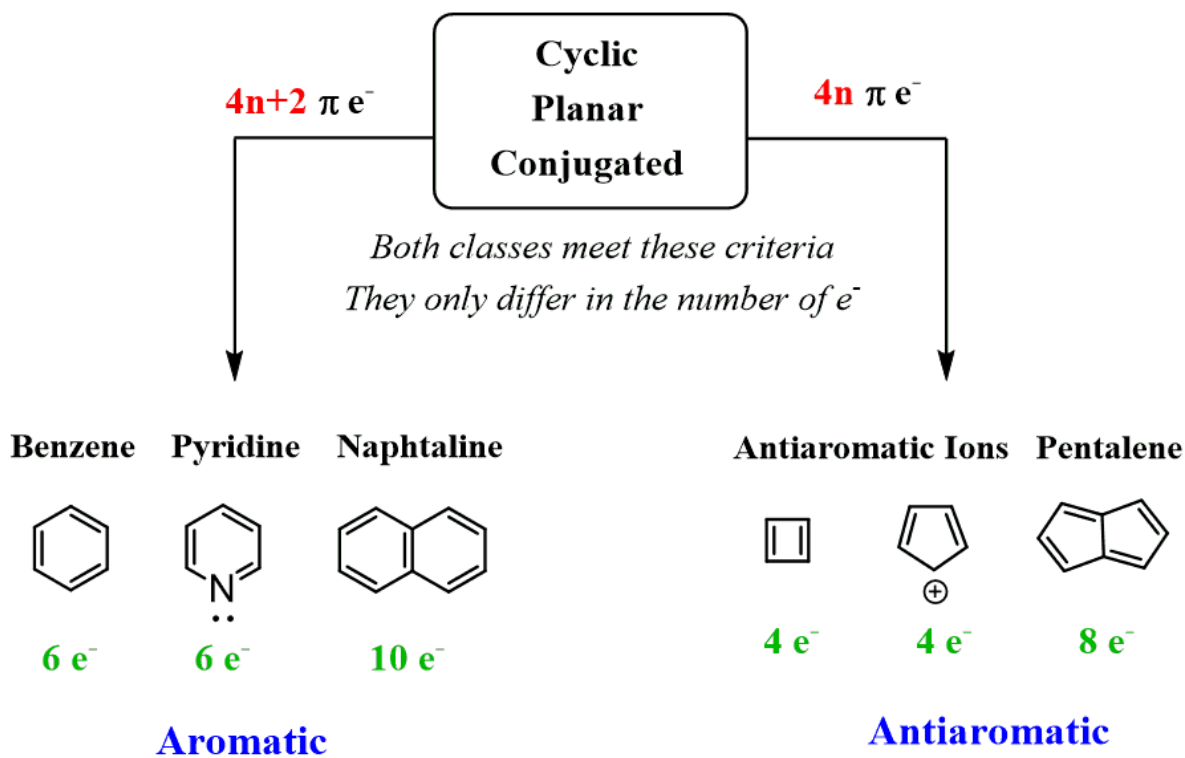
$$n = 1$$

An aromatic compound follows Huckel's rule if n is equal to zero or a positive whole number.

Benzene is aromatic

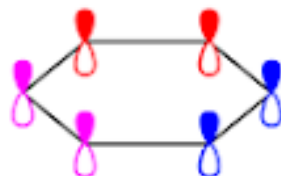
1.2 Classification of aromatic compound

Classification of Aromatic and Antiaromatic Compounds



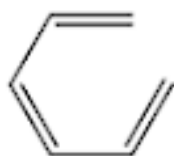


benzene

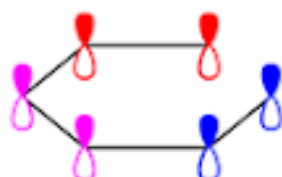


1. Cyclic
2. *p*-orbital for each member of the ring
3. Planar ring (sp^2 hybridized)
4. $4n+2$ π -bond electron count.

Aromatic



hexatriene

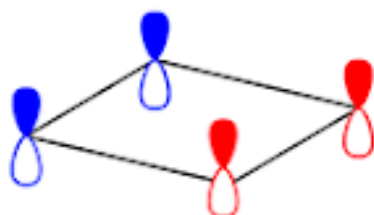


1. **NOT Cyclic**
2. *p*-orbital for each member of the ring
3. Planar ring (sp^2 hybridized)
4. $4n+2$ π -bond electron count.

Non-Aromatic



cyclobutadiene



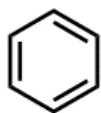
1. Cyclic
2. *p*-orbital for each member of the ring
3. Planar ring (sp^2 hybridized)
4. **Closed** $4n$ π -bond electron count.

Anti-Aromatic

Four Rules For Aromaticity

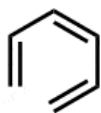
Condition #1: The molecule must be cyclic

No exceptions!



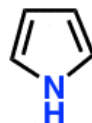
cyclic

Benzene
Aromatic



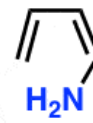
acyclic

(Z)-1,3,5 hexatriene
Not aromatic



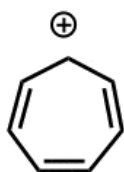
cyclic

Pyrrole
Aromatic



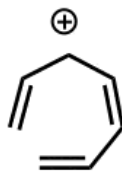
acyclic

Not aromatic



cyclic

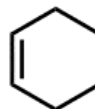
"Tropylium" ion
Aromatic



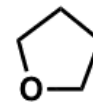
acyclic

Not aromatic

*Just to be clear: not all
cyclic molecules are aromatic...*



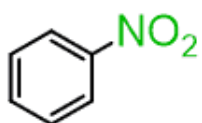
cyclohexene
(not aromatic)



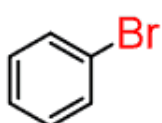
tetrahydrofuran
(not aromatic)

1.3 Nomenclature of aromatic compounds

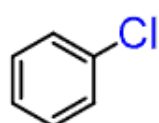
common names



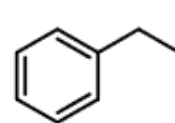
nitrobenzene



bromobenzene

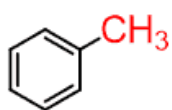


chlorobenzene

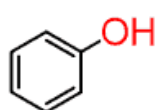


ethylbenzene

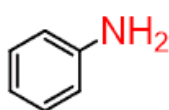
Common IUPAC names of monosubstituted aromatic compounds



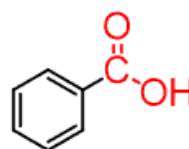
Toluene



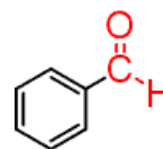
Phenol



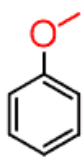
Aniline



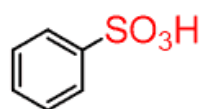
Benzoic acid



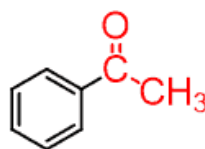
Benzaldehyde



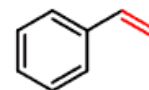
Anisole



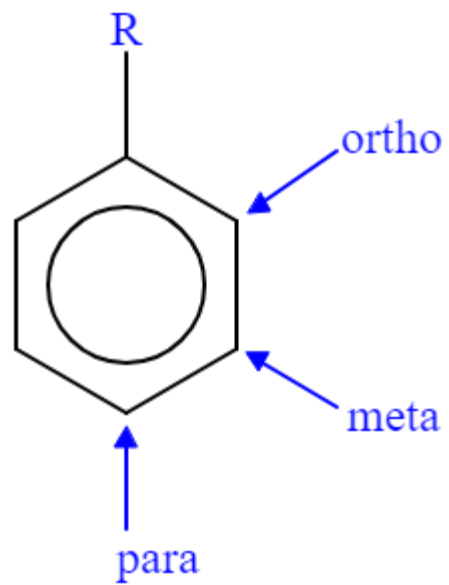
Benzenesulfonic acid



Acetophenone



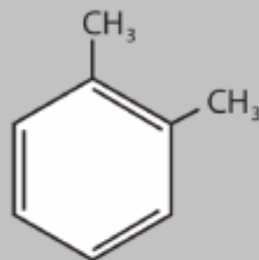
Styrene



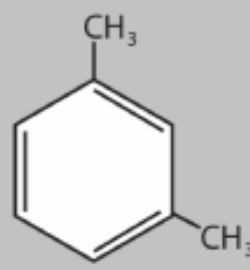
Benzene



Toluene



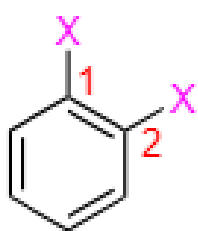
Ortho-xylene



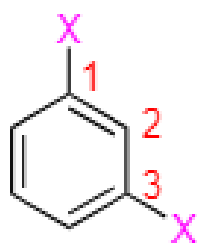
Meta-xylene



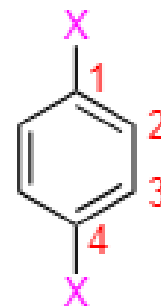
Para-xylene



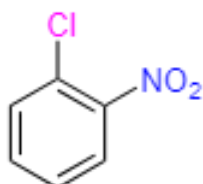
ortho-Disubstituted
(1,2)



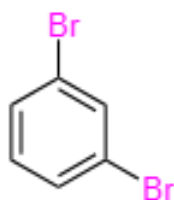
meta-Disubstituted
(1,3)



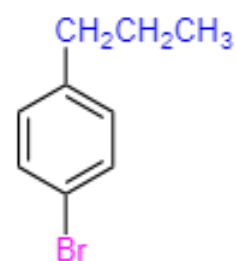
para-Disubstituted
(1,4)



ortho-Chloronitrobenzene



meta-Dibromobenzene



para-Bromopropylbenzene