

**B.Sc. Semester-VI
Organic Chemistry
Paper-XIV**



3. Heterocyclic Compounds

Coverage:

2. Orbital Picture and Aromatic Characteristics of Heterocyclic Compounds



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Orbital Picture and Aromatic Characteristics of Heterocyclic Compounds

To be classified as aromatic, a compound must have:

1. Cyclic structure
2. Coplanar structure.
3. Each atom of the ring must have a p orbital to form a delocalized π system i.e. no atoms in the ring can be sp^3 hybridized instead all atoms must be sp^2 hybridized.

Conjugated C=C bonds (C=C-C=C-C=C)

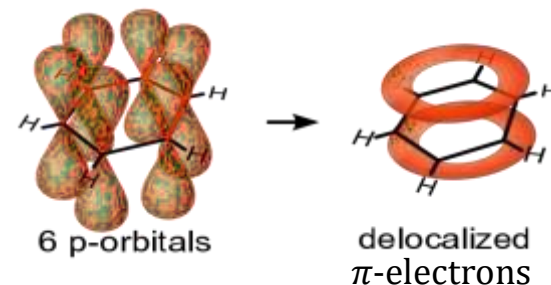
4. Fulfill Huckel rule i.e. the system must have

$4n + 2 \pi$ Electrons

thus by calculating n value it will be an integral number i.e. $n=0, 1, 2, 3,$

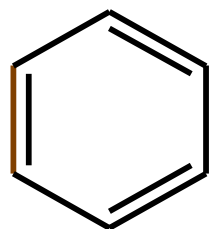


Erich Hückel

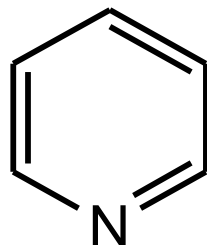


Examples of Aromatic and Non-Aromatic Compounds

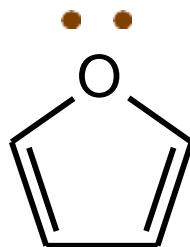
Examples of aromatic compounds:



$n=1$



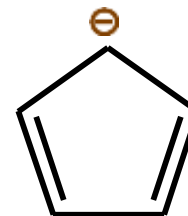
$n=1$



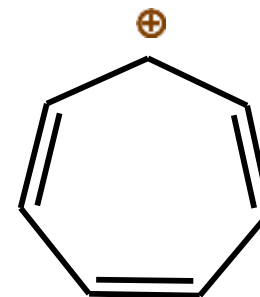
$n=1$



$n=0$

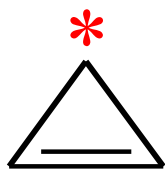


$n=1$

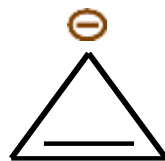


$n=1$

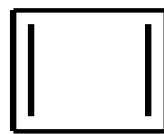
Examples of non-aromatic compounds:



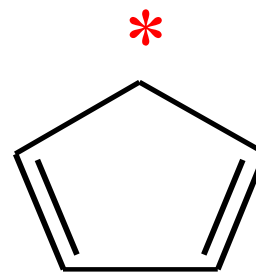
$sp^3 C^*$



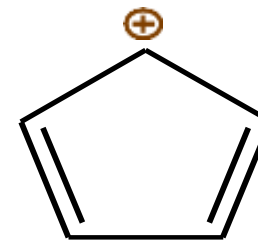
$n=1/2$



$n=1/2$

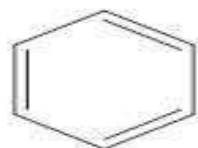


$sp^3 C^*$



$n=1/2$

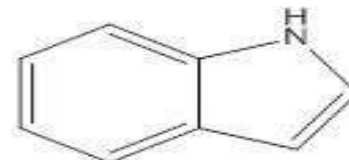
Examples of Aromatic and Non-Aromatic Compounds



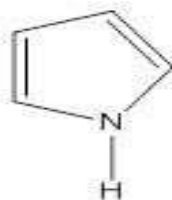
$$4n + 2 = 6$$
$$n = 1$$



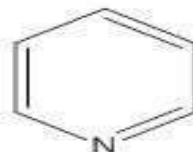
$$4n + 2 = 10$$
$$n = 2$$



$$4n + 2 = 6$$
$$n = 1$$



$$n = 1$$



$$n = 1$$



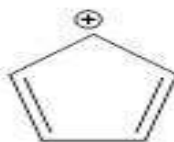
$$4n + 2 = 4$$
$$n = 1$$



$$4n + 2 = 2$$
$$n = 0$$

Aromatic

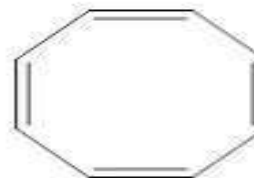
But



$$4n + 2 = 4$$
$$n \neq 1$$



$$4n + 2 = 4$$
$$n \neq 1$$



$$4n + 2 = 8$$

is not an integer

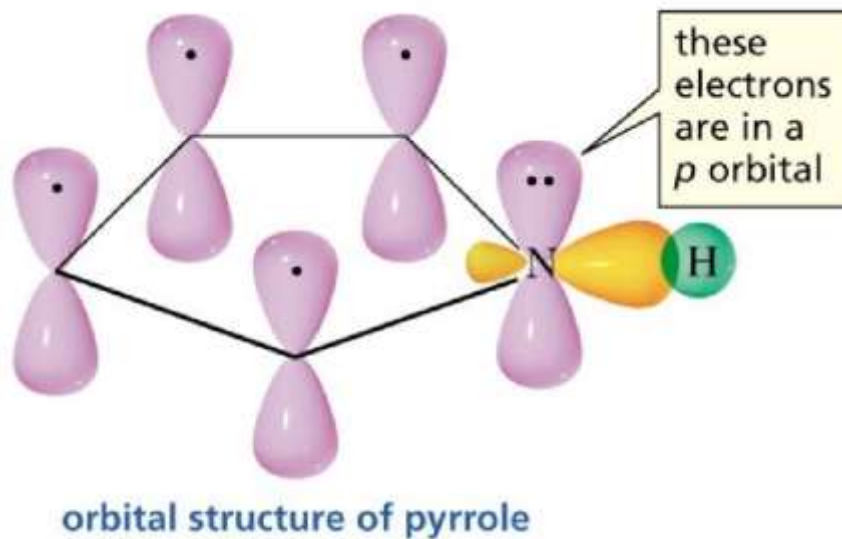
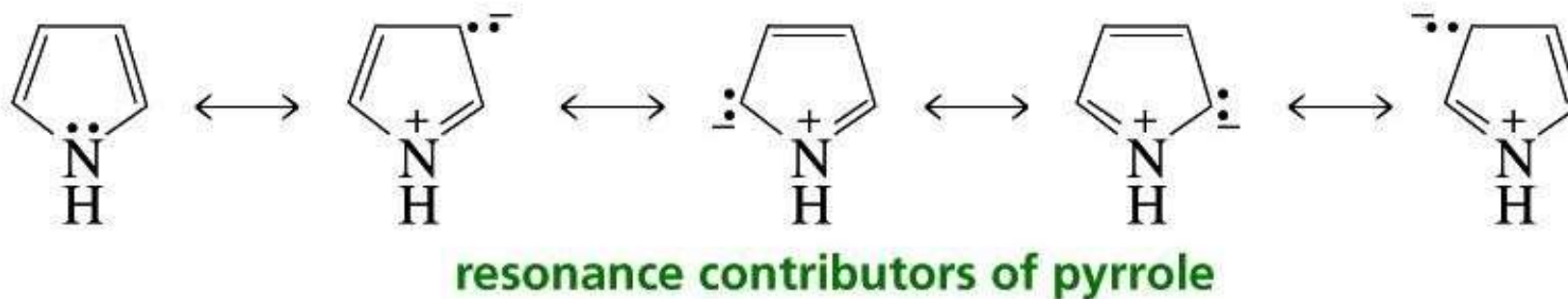


$$4n + 2 = 4$$
$$n \neq 0$$

not aromatic

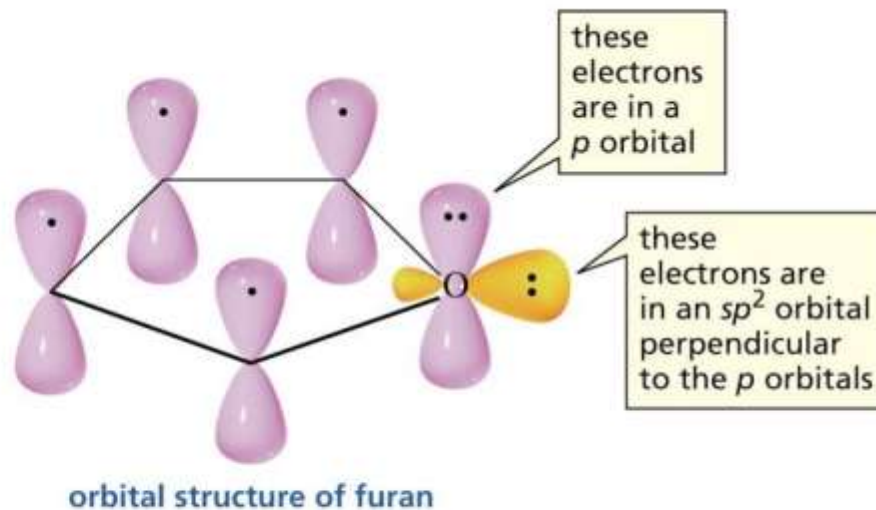
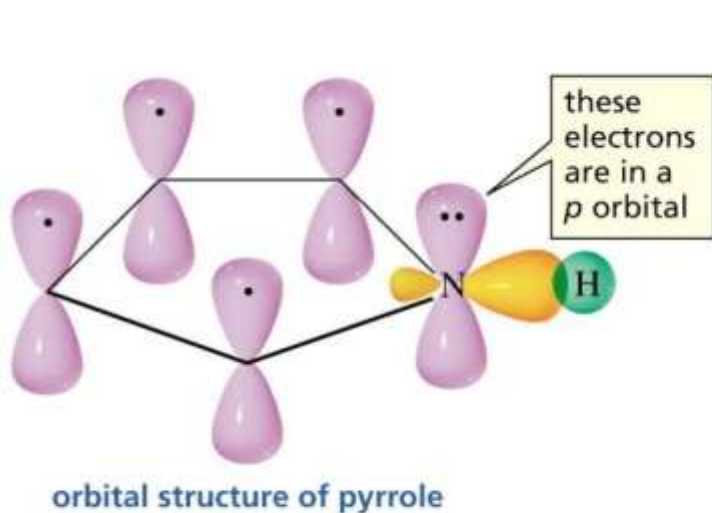
Orbital Picture and Aromatic Characteristics of Pyrrole

Pyrrole is Aromatic



Orbital Picture and Aromatic Characteristics of Furan

Furan is Aromatic



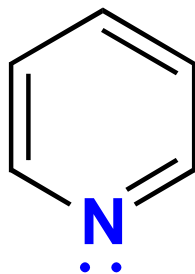
Orbital Picture and Aromatic Characteristics of Pyridine

Heterocyclic Aromatic Compounds and Hückel's Rule:

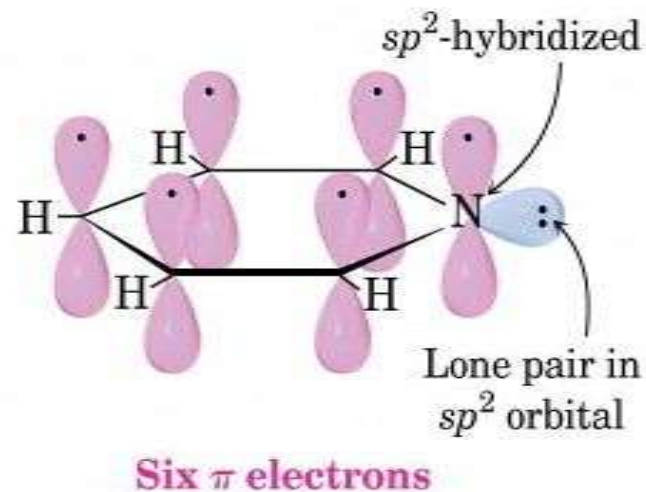
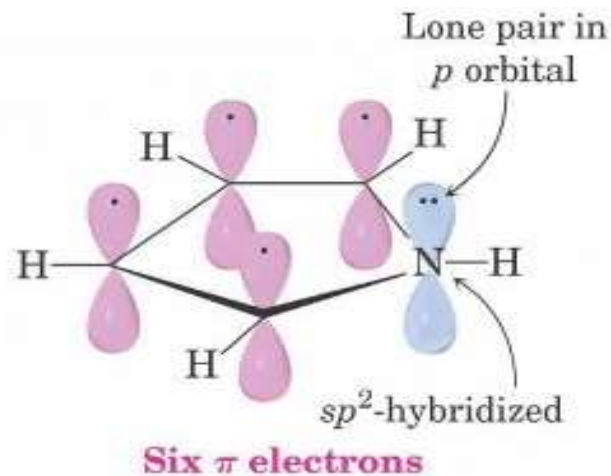
Pyridine: π -electron structure resembles benzene (6 π -electrons) The nitrogen lone pair electrons are not part of the aromatic system.

But in pyrrole, lone pair of electrons is delocalized in the ring.

Pyridine is Aromatic

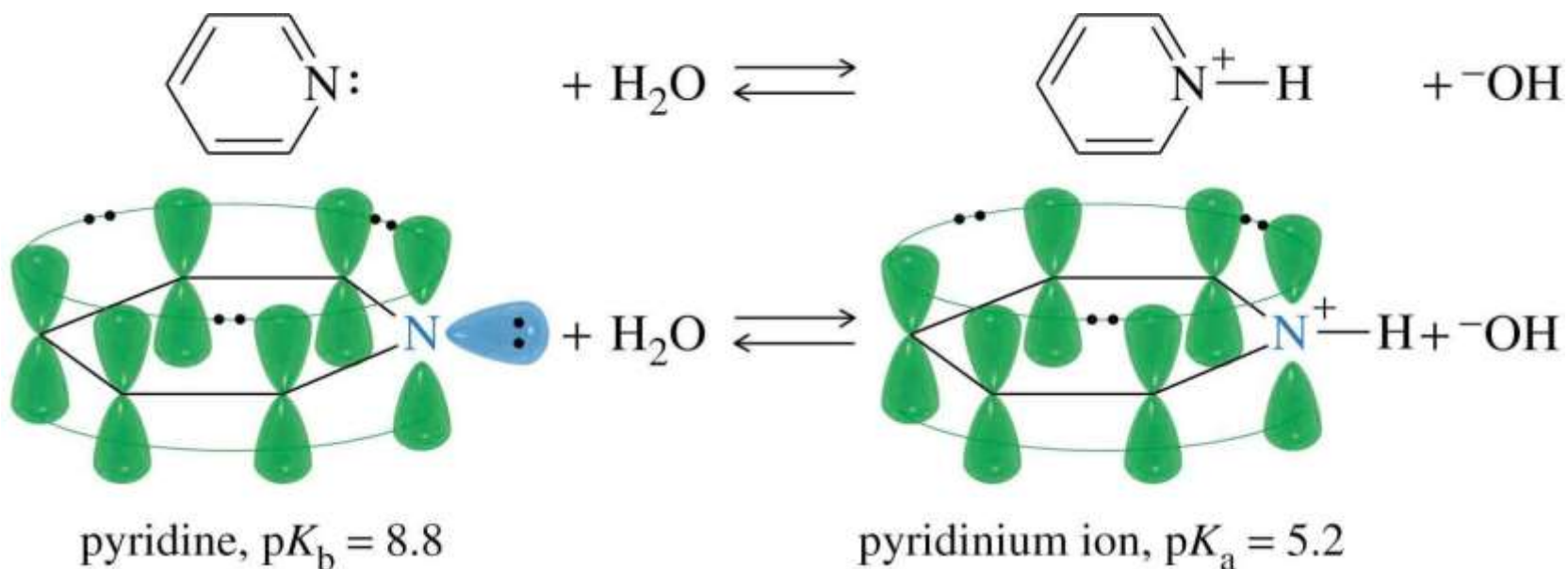


pyridine



The Acidity of the Pyridinium Ion

- Heterocyclic aromatic compound.
- Nonbonding pair of electrons in sp^2 orbital, so weak base, $pK_b = 8.8$.



The Acidity of Protonated Pyrrole

Also aromatic, but lone pair of electrons are delocalized:
Much weaker base.

