

M.Sc. Semester-I
Core Course-II (CC-II)
Reaction Mechanism in Organic Chemistry



I. Nature of Bonding in Organic Molecules

L2. Aromaticity in Benzenoid and Non-benzenoid Compounds



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Hückel's Rule:

Aromatic:

Cyclic

Conjugated: “alternating single and double bonds”

Planar: maximum overlap between conjugated π -bonds **Must contain $4n+2$ π -electrons, where n is an integer.**

Anti-aromatic:

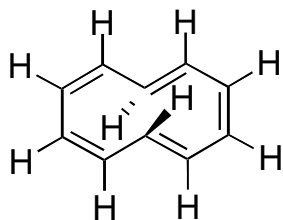
cyclic, conjugated, planar molecules that contain $4n$ π -electrons (where n is an integer).

Destabilized (highly reactive) relative to the corresponding open-chain conjugated system

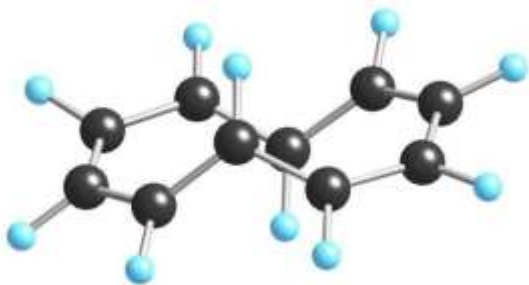
Cyclic Conjugation is necessary, but not sufficient criteria for aromaticity.

Annulenes - monocyclic, conjugated, planar polyenes that conform to Hückel's rule

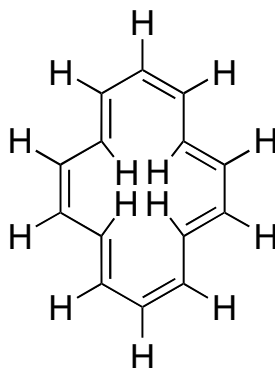
[10]annulene



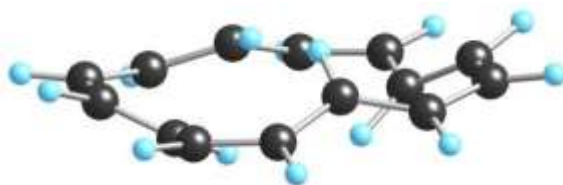
10 π -electrons
 $4n+2 = 10, n=2$.



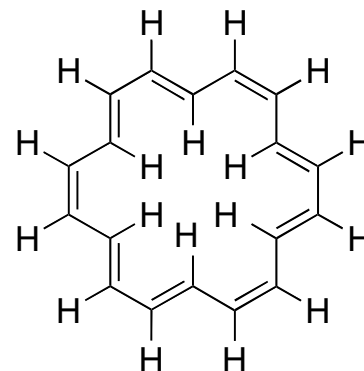
[14]annulene



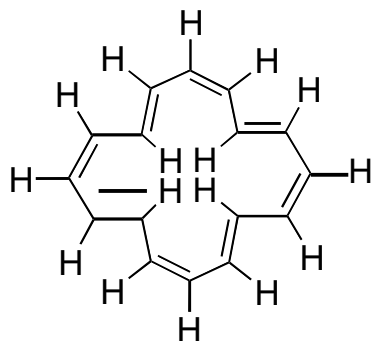
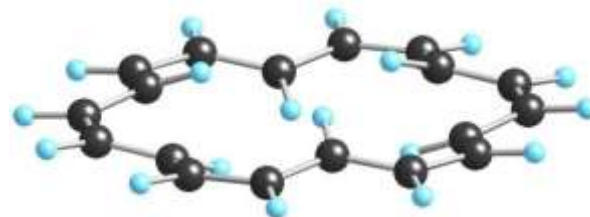
14 π -electrons
 $4n+2=14, n=3$



[18]annulene

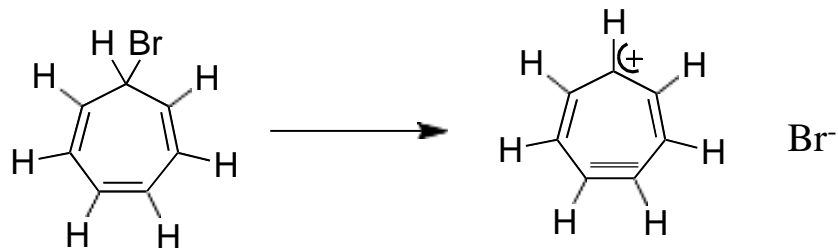
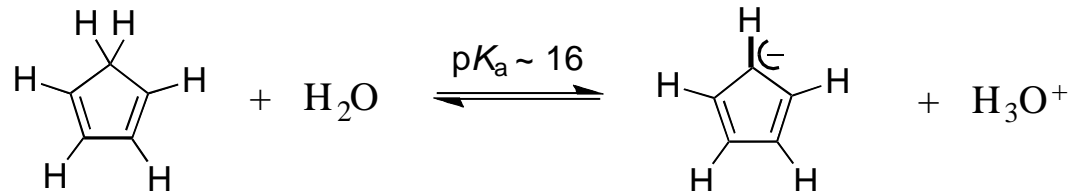
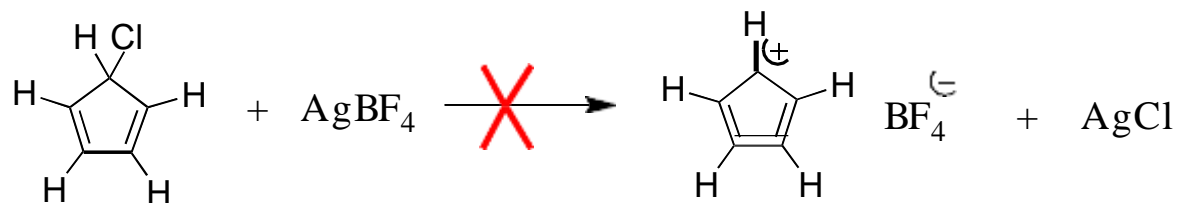
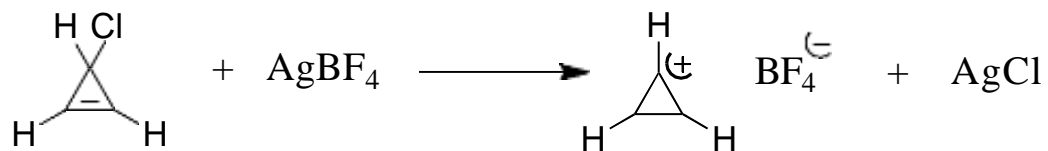


18 π -electrons
 $4n+2=18, n=4$

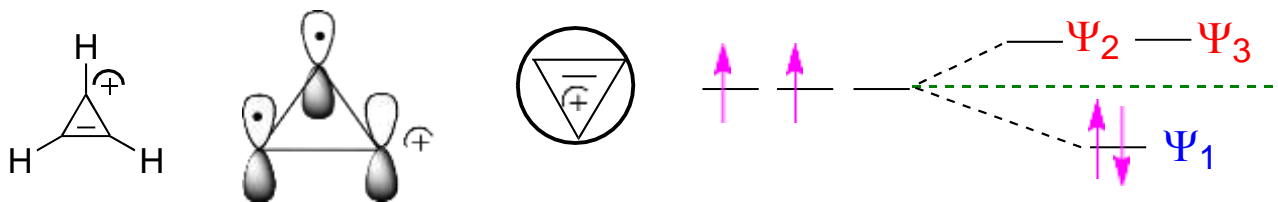


[16]annulene
16 π -electrons
 $4n=16, n=4$

Aromatic Ions



Cyclopropenyl cation



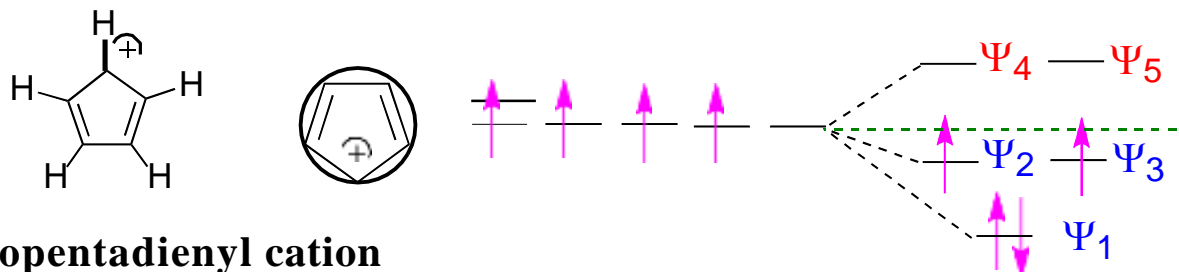
cyclopropenyl cation
2 π -electrons

$$4n+2=2$$

$$n=0$$

aromatic

Cyclopentadienyl cation



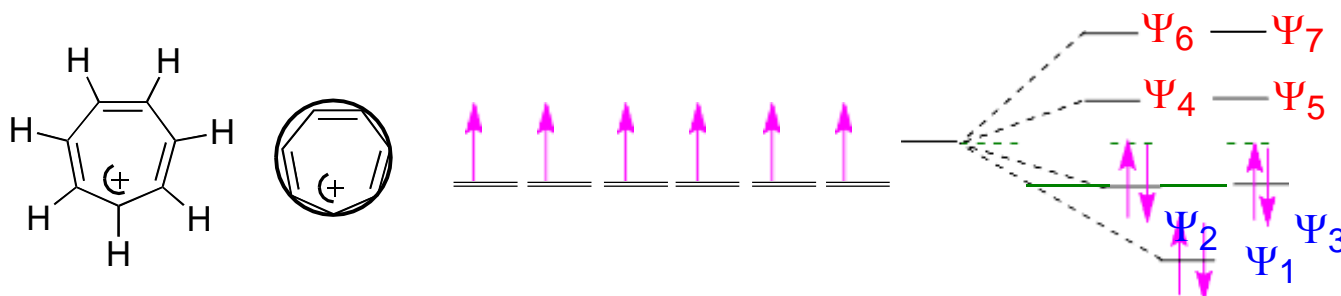
cyclopentadienyl cation
4 π -electrons

$$4n=4$$

$$n=1$$

anti-aromatic

Cycloheptatrienyl cation



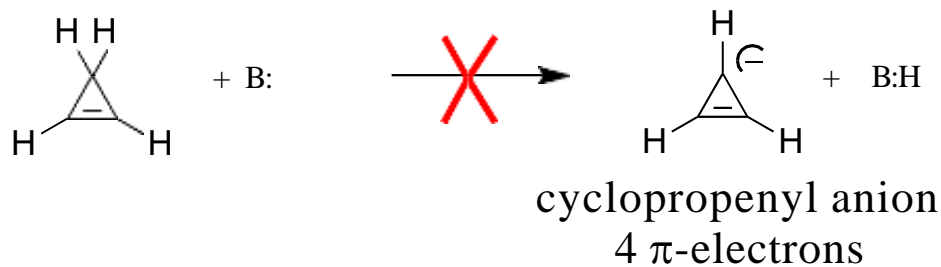
Cycloheptatrienyl cation
6 π -electrons

$$4n+2=6$$

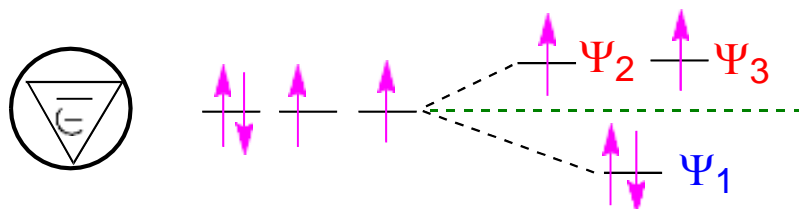
$$n=1$$

aromatic

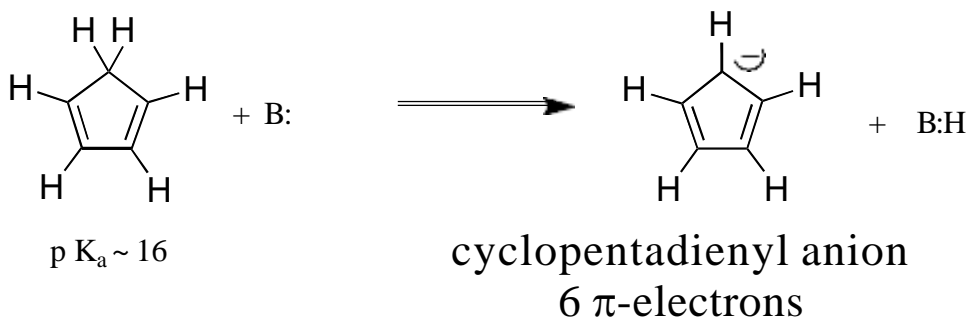
Cyclopropenyl anion



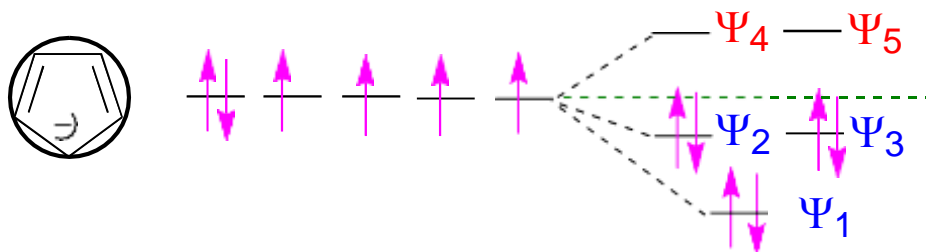
$4n=4$
 $n=1$
 anti-aromatic



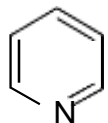
Cyclopentadienyl anion



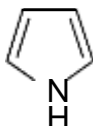
$4n+2=6$
 $n=1$
 aromatic



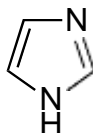
Heterocyclic Aromatic Compounds : Any cyclic compound that contains ring atom(s) other than carbon (N, O, S, P). Cyclic compounds that contain only carbon are called carbocycles.



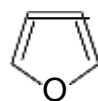
pyridine



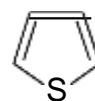
pyrrole



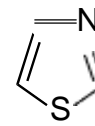
imidazole



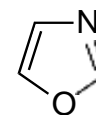
furan



thiophene



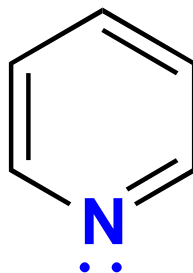
thiazole



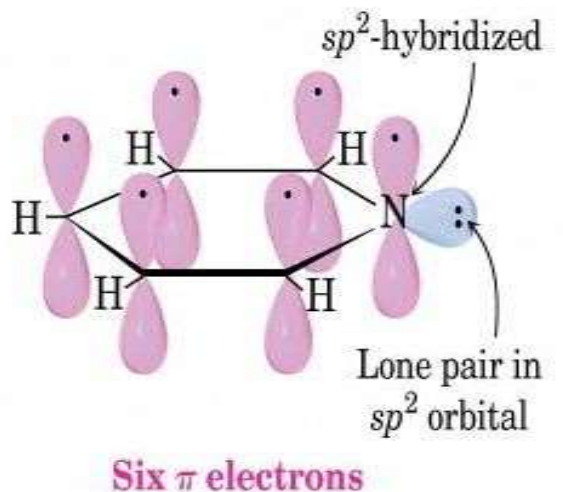
oxazole

Heterocyclic Aromatic Compounds and Hückel's Rule:

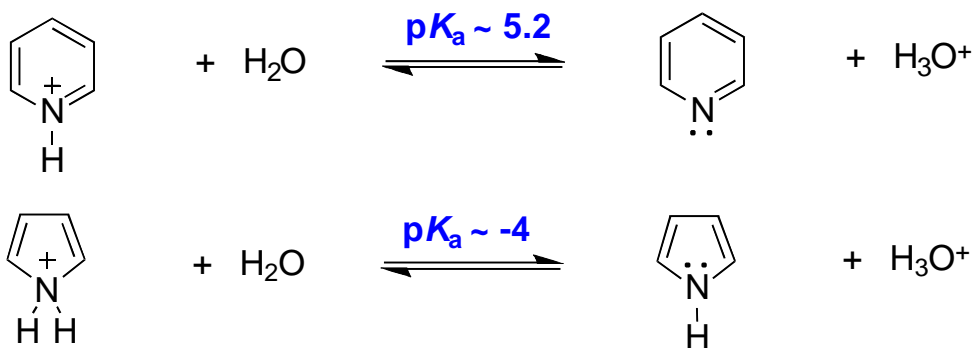
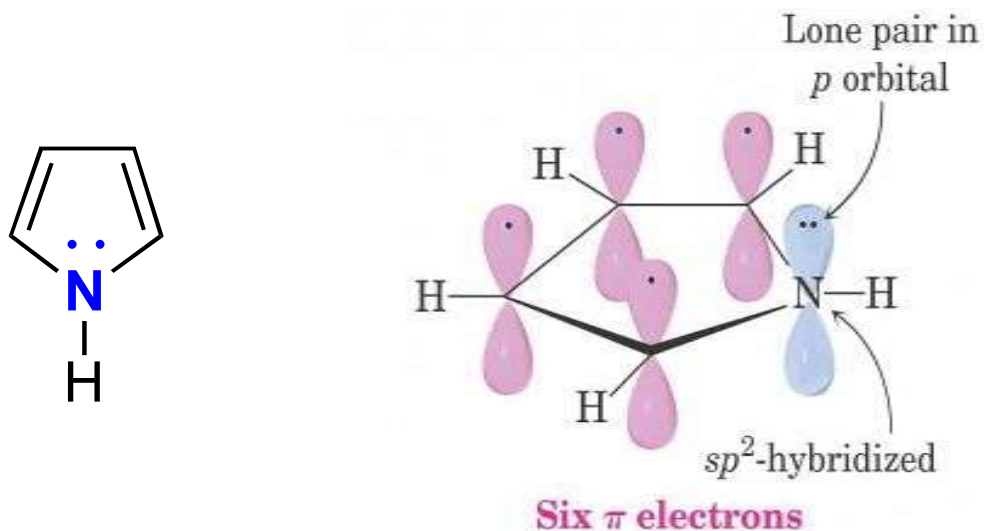
Pyridine: π -electron structure resembles benzene (6 π -electrons) The nitrogen lone pair electrons are not part of the aromatic system.



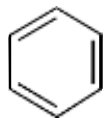
pyridine



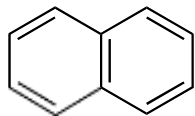
Pyrrole: 6 π -electron system similar to that of cyclopentadienyl anion. There are four sp^2 -hybridized carbons with 4 p orbitals perpendicular to the ring and 4 π -electrons and a lone pair of electrons in an unhybridized p^2 orbital that is part of the aromatic sextet.



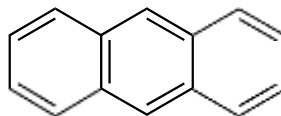
Polycyclic Aromatic Hydrocarbons (PAHs) : $4n+2$ System



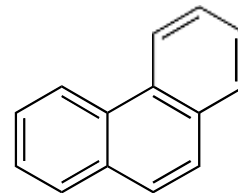
benzene



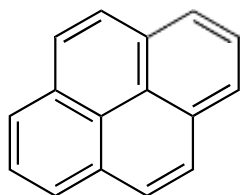
naphthalene



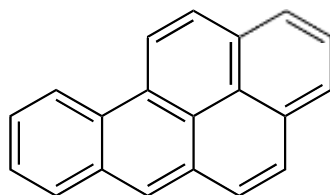
anthracene



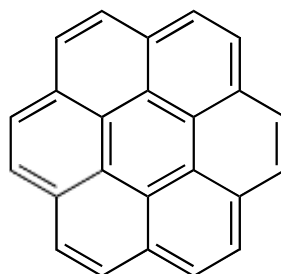
phenanthrene



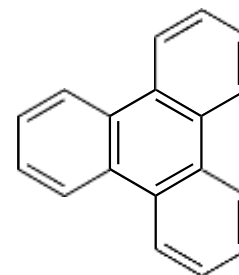
pyrene



benzo[a]pyrene



coronene



triphenylene

Thank You



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