**B.Sc. Semester-II**
**Core Course-III (CC-III)**
**Organic Chemistry-I**

# IV. Aromatic Hydrocarbons

## 3. Hückel's Rule

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**Dr. Shyama Prasad Mukherjee University, Ranchi**

**IV Aromatic Hydrocarbons** **10 Lectures**

Aromaticity: Hückel's rule, aromatic/anti-aromatic/non-aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples.

Electrophilic aromatic substitution: Halogenation, Nitration, Sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of mono-functional groups.

**Coverage:**

1. Hückel's Rule
2. Aromatic/anti-aromatic/non-aromatic character of cyclic carbocations/ carbanions and heterocyclic compounds with suitable examples

**Hückel's Rule:**

**Aromatic:**

**Cyclic**

**Conjugated: "alternating single and double bonds"**

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

**Anti-aromatic:**

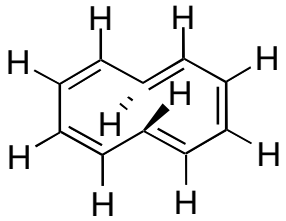
**cyclic, conjugated, planar molecules that contain 4n $\pi$-electrons (where n is an integer).**

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

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

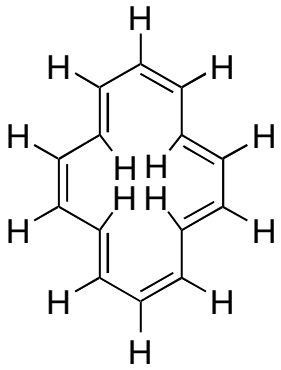
**Annulenes - monocyclic, conjugated, planar polyenes that conform to Hückel's rule**

**[10]annulene**



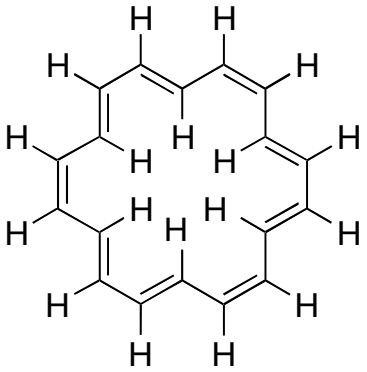
**10 π-electrons**
**4n+2 = 10, n=2.**

**[14]annulene**

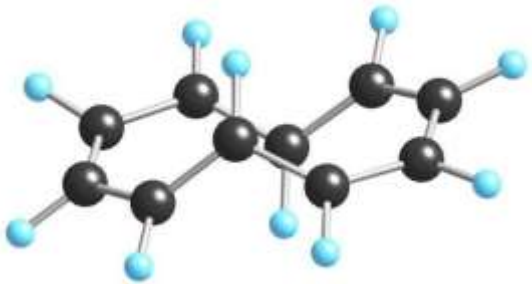


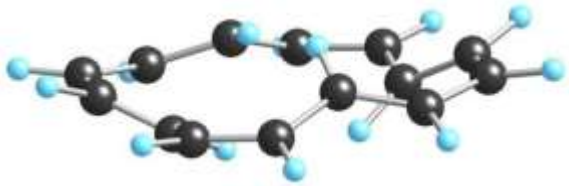
**14 π-electrons**
**4n+2=14, n=3**

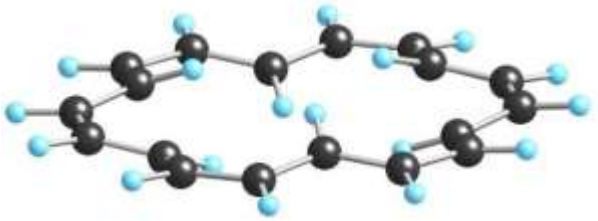
**[18]annulene**

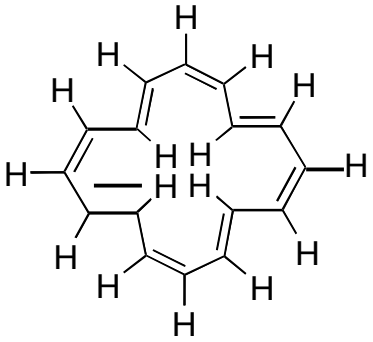


**18 π-electrons**
**4n+2=18, n=4**



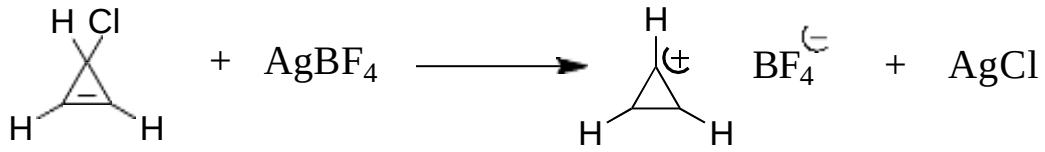


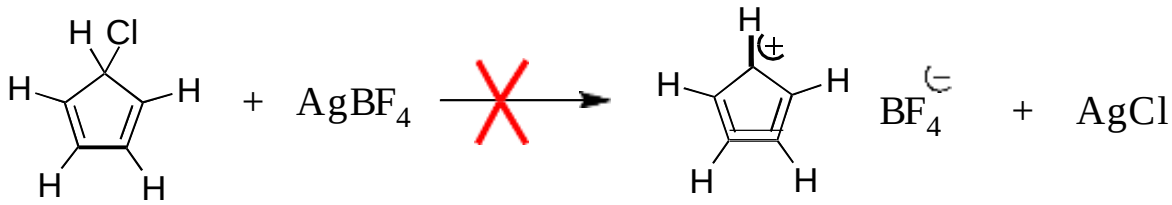


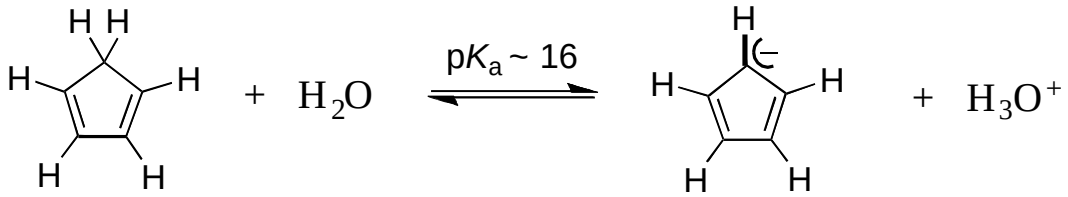


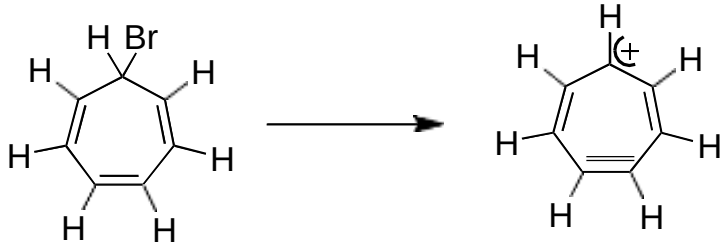
**[16]annulene**
**16 π-electrons**
**4n=16, n=4**

## Aromatic Ions

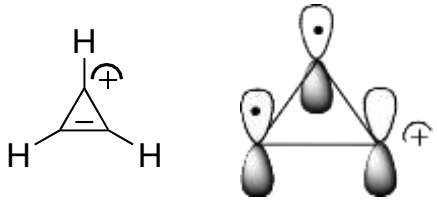


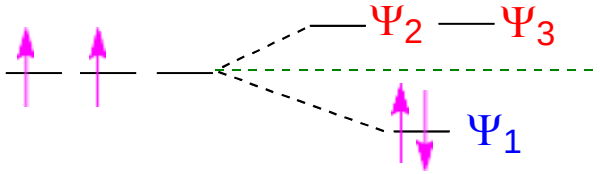



## Cyclopropenyl cation



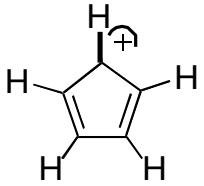


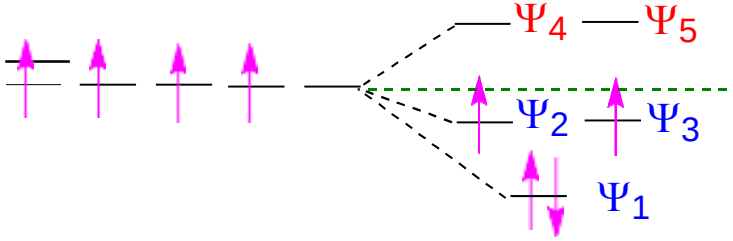




cyclopropenyl cation
2 π-electrons

**4*n*+2=2**
***n*=0**
**aromatic**

## Cyclopentadienyl cation



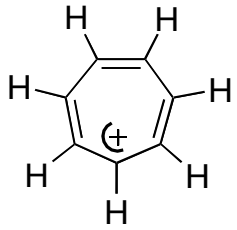



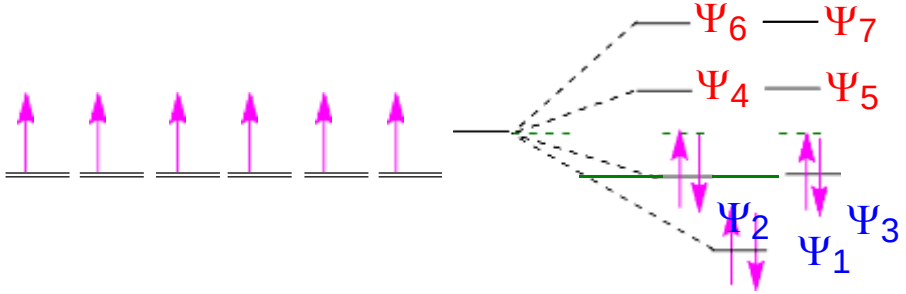

cyclopentadienyl cation

4 π-electrons

**4*n*=4**
***n*=1**
**anti-aromatic**

## Cycloheptatrienyl cation

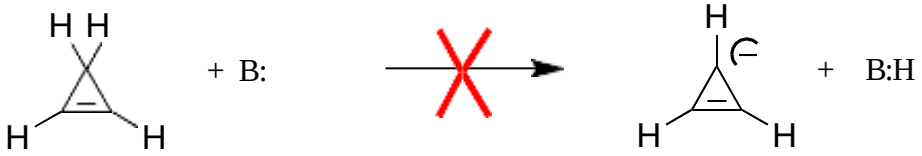



Cycloheptatrienyl cation
6 π-electrons

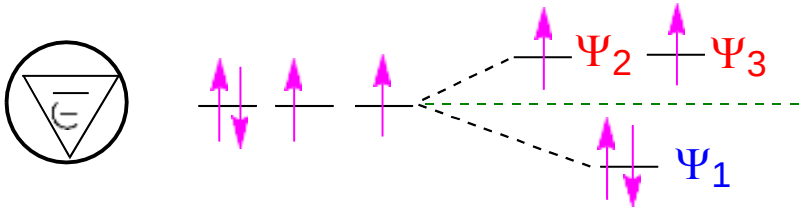
**4n+2=6**
***n*=1**
**aromatic**

## Cyclopropenyl anion

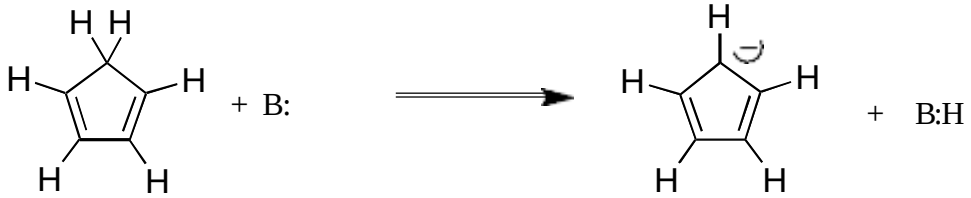



cyclopropenyl anion
4 π-electrons

**4*n*=4**
***n*=1**
**anti-aromatic**



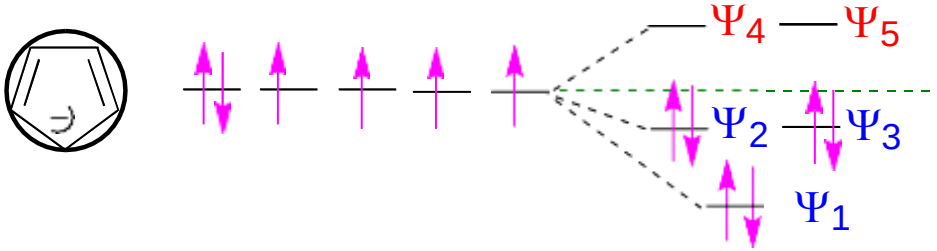

## Cyclopentadienyl anion



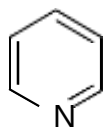

p $K_a$ ~ 16

cyclopentadienyl anion
6 π-electrons

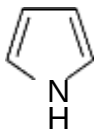
**4*n*+2=6**
***n*=1**
**aromatic**



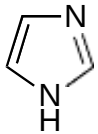
**Heterocyclic Aromatic Compounds (please read)** **Heterocycle: any cyclic compound that contains ring atom(s) other than carbon (N, O, S, P). Cyclic compounds that contain only carbon are called carbocycles.**



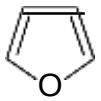

**pyridine**



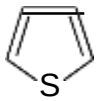

**pyrrole**



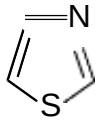

**imidazole**



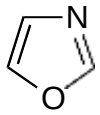

**furan**




**thiophene**



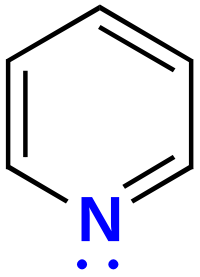

**thiazole**



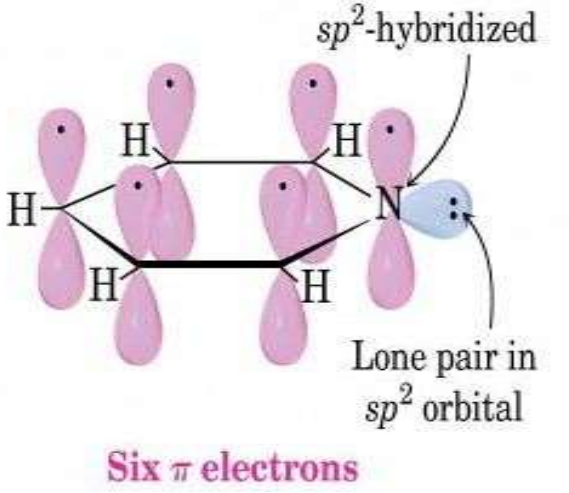

**oxazole**

**Heterocyclic Aromatic Compounds and Hückel's Rule:**

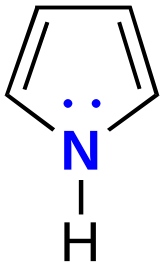
**Pyridine: π-electron structure resembles benzene (6 π-electrons) The nitrogen lone pair electrons are <u>not</u> part of the aromatic system.**

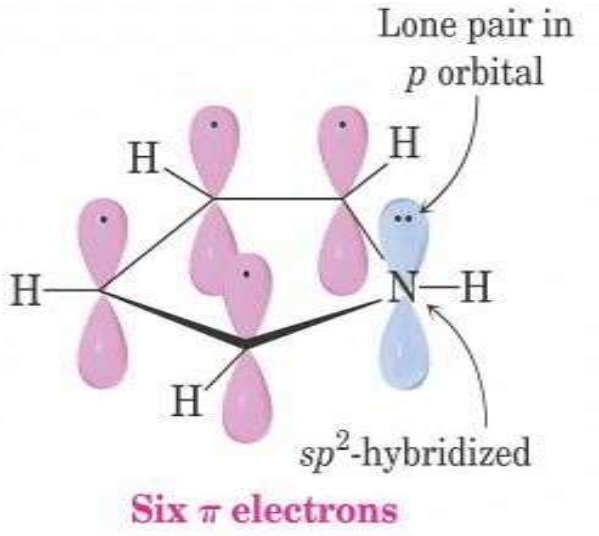


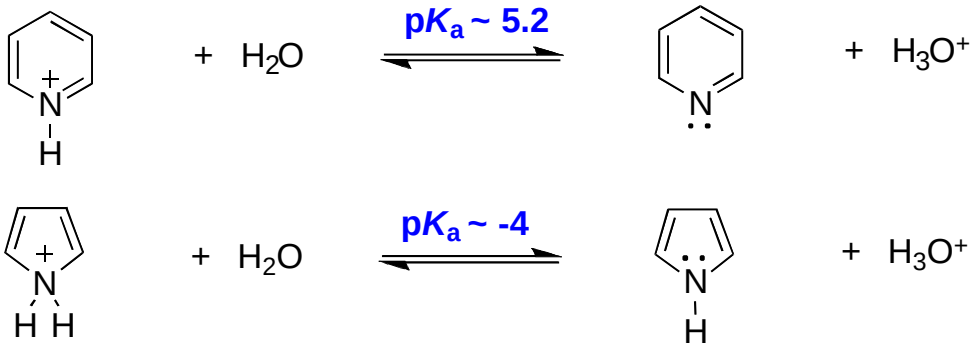

pyridine



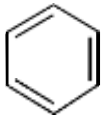
**Pyrrole: 6 π-electron system similar to that of cyclopentadienyl anion. There are four *sp*²-hybridized carbons with 4 *p* orbitals perpendicular to the ring and 4 π-electrons and a lone pair of electrons in an unhybridized p² orbital that is part of the aromatic sextet.**



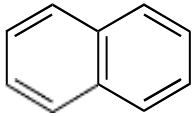


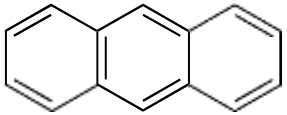
## Polycyclic Aromatic Hydrocarbons (PAHs) : 4n+2 System



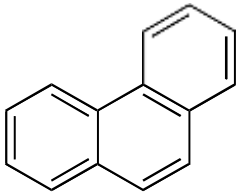
**benzene**



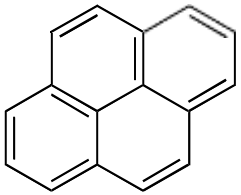
**naphthalene**



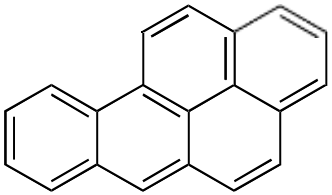
**anthracene**



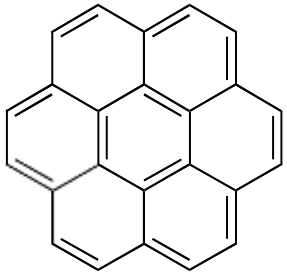
**phenanthrene**



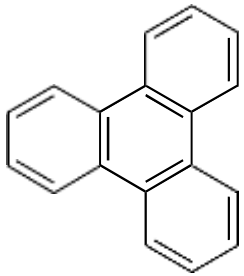
**pyrene**



**benzo[a]pyrene**

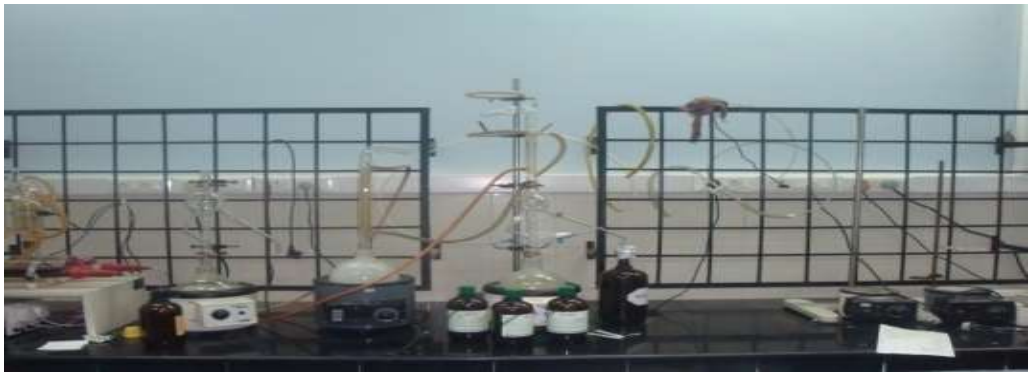


**coronene**



**triphenylene**

# Thank You



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