

ARENS AND AROMATICITY

Huckel rule or $(4n+2)\pi$ rule.

German scientist Huckel made a remarkable contribution to the structural organic chemistry. On the basis of certain molecular orbital calculations, he suggested the criterion for exhibition of aromatic properties by a given ring system which is known as Huckel rule or $(4n+2)\pi$ rule of aromaticity.

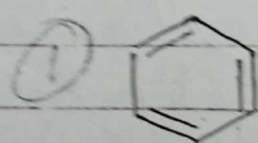
The main theoretical requirements for a species to possess aromaticity are:

- 1) The molecule or ion must be planar, cyclic and planar.
- 2) It must have cyclic clouds of delocalised π -electrons above and below the plane of the molecule or ion.
- 3) The π -electron cloud in the molecule or ion must contain a total of $(4n+2)\pi$ electrons. where $n = 0, 1, 2, \dots$

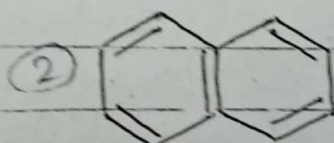
Ex. 1. Benzene:

Thus according to Huckel rule benzene is aromatic because it is cyclic, planar, and conjugated and containing ~~6 π ele~~ 6π -electrons.

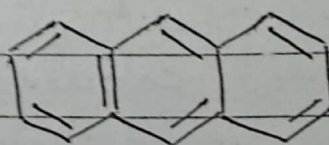
Aromatic molecules:



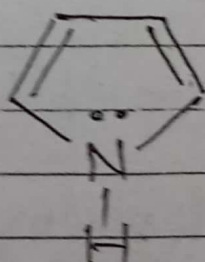
Benzene
 $n=1$
(6π -electrons)



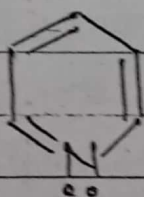
Naphthalene
 $n=2$
 10π electrons.



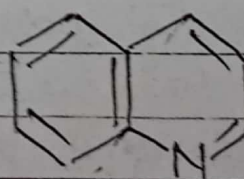
Anthracene
 $n=3$
 14π electrons.



Pyrrole
 $n=1$
 6π electrons.

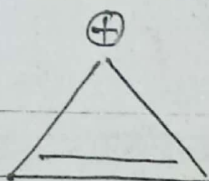


Pyridine
 $n=1$
 6π electrons.

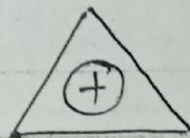


Quinoline
 $n=2$
 10π electrons.

Aromatic ions:



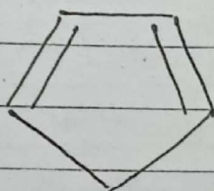
or



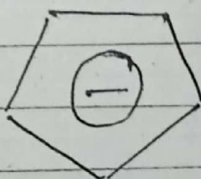
$$n = 0$$

2π -electrons.

cyclopropenyl cation



or



$$n = 2$$

6π -electrons.

cyclopentadienyl anion.

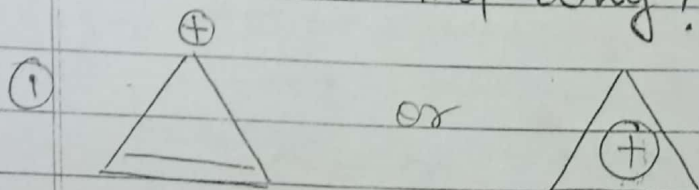
Limitations of Huckel rule:

There are two important limitations of Huckel rule

- i/ It is not necessary and sufficient condition for aromaticity and
- ii, Huckel's rule predicts whether a compound or a system would be aromatic or not, but it does not indicate the relative degree of aromaticity in isoelectronic systems.

It should be noted that there exist compounds which do not contain $(4n+2)\pi$ electrons, yet are not aromatic. For example [10] annulenes, [14] annulene etc. Further there

Q. Which of the following compounds are aromatic and why?



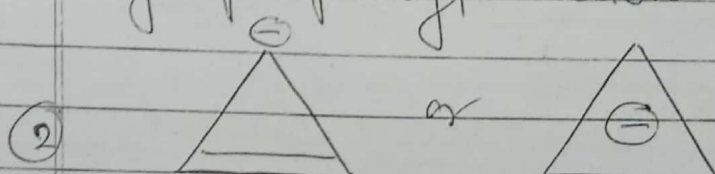
Cyclopropenyl cation

$$n = 0$$

No. of π -electrons = 2

\therefore Aromatic. $n = 0$

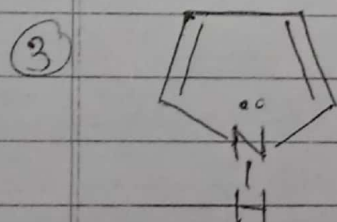
Thus cyclopropenyl cation is aromatic



Cyclopropenyl anion

No. π -electrons = 4

There is no permissible n .
Thus it is nonaromatic.

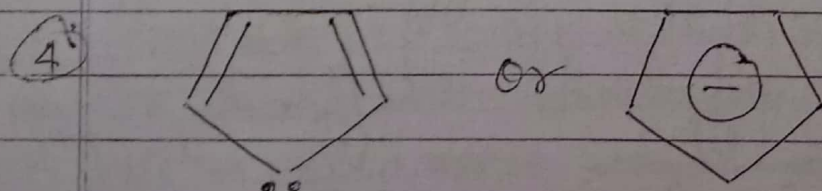


No. of π -electrons = 6

$\therefore n = 1$

Thus it is aromatic.

Pyrrole



Cyclopentadienyl anion

$$n = 1$$

No. of π -electrons = 6

$\therefore n = 1$

Thus it is aromatic.