AROMATICITY

Huckel's Rule

In 1931, the German physicist Erich Hückel carried out a series of mathematical calculations to furnish a rule for the prediction of aromaticity.

According to this rule, planar monocyclic rings containing $(4n+2)$ π electrons, where $n = 0, 1, 2, 3 - \ldots$, have closed shell of delocalized electrons and should be aromatic.

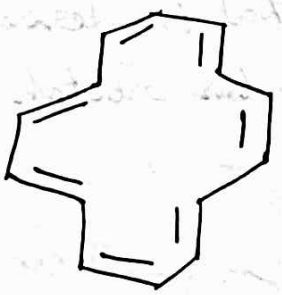
Therefore, benzene is aromatic because it has 6 π electrons ($n = 1$) where as cyclooctatetraene having 8 π electrons does not obey Huckel's rule and is not aromatic..

Benzene
(6 π electrons)
($n = 1$ for Huckel's $(4n+2)$ π electron rule)

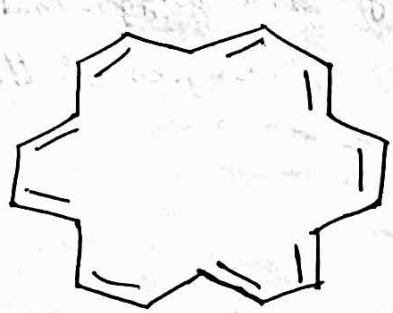
Cyclooctatetraene
(8 π electrons)
(Not aromatic)

According to Huckel's rule, rings containing 2, 6, 10, 14, 18, - ... π electrons are aromatic.

For example —



[14] Annulene
Aromatic, because
$n = 3$ for Huckel's
$(4n+2)$ π electron rule



[18] Annulene
Aromatic, because
$n = 4$ for Huckel's $(4n+2)$ π
electron rule

The Rules for Aromaticity

1. The molecule must be cyclic, with conjugated π-bonds and planar (or nearly planar).
2. The ring atoms are usually sp^2 hybridized or occasionally sp hybridized. So, each atom in the ring must have an unhybridized p-orbital.
3. The unhybridized p-orbitals must overlap to form a continuous ring of ~~parrot~~ parallel orbitals.
4. For cyclic system to be aromatic, it will contain ~~4n+~~ $(4n+2)\pi$ electrons, where n is an integer, 0, 1, 2, 3.....
5. Whether a compound is aromatic or not, can be determined from ^{1}HNMR spectrum. If the protons attached to the ring are shifted downfield from the normal olefinic region, then the compound is diatropic and aromatic.

   Thus compared to ordinary olefinic Hs which are found around 5-6 δ, the Hs of the benzene ring are located around 7-8 δ.

Annulenes

The name annulene has been proposed as a general name for monocyclic compounds that can be represented by structures having alternating single and double C-C bonds.

The ring size of an annulene is indicated by a number in brackets.

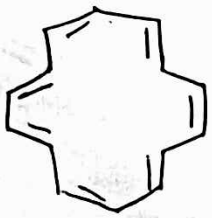
Example

Benzene is [6] annulene and cyclooctatetraene is [8] annulene.

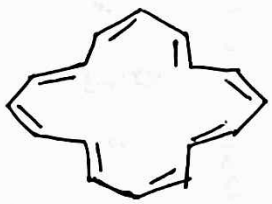
Benzene
([6] annulene)

cyclooctatetraene
([8] annulene)

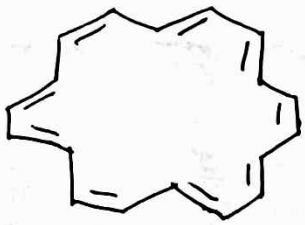
Some examples of Annulenes:-



[14] Annulene



[16] Annulene



[18] Annulene