B.Sc. (Honours) Part-III

Paper-I (General)

Topic: Huckel's rule

UG
Subject-Chemistry

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Huckel's Rule: The 4n+2π Electron Rule

Huckel's Rule is used in order to estimate the aromatic qualities of any planar ring-shaped molecule in the field of organic chemistry. The supporting quantum mechanics required for the formulation of this rule was solved first by the German physical chemist and physicist Erich Armand Arthur Joseph Huckel in the year 1931.

➔ **Planar monocyclic rings with a continuous system of *p* orbitalsand 4n + 2π electrons are aromatic (n = 0, 1, 2, 3 etc)**

Aromatic compounds have substantial resonance stabilization

Benzene is aromatic: it is planar, cyclic, has a *p* orbital at every carbon, and 6 □ electrons (n=1)

➔ **There is a *polygon-and-circle method* for deriving the relative energies of orbitals of a system with a cyclic continuous array of *p* orbitals**

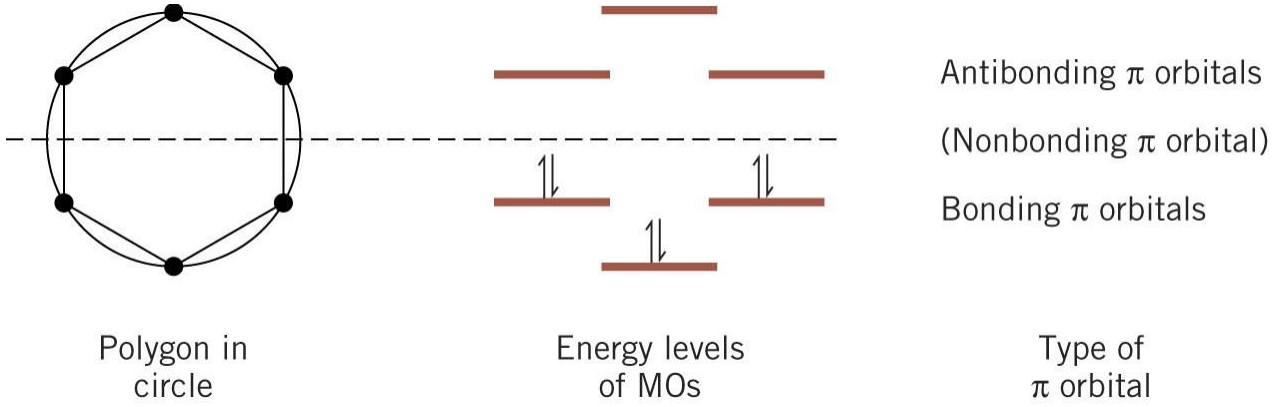
A polygon corresponding to the ring is inscribed in a circle with one point of the polygon pointing directly down

A horizontal line is drawn where vertices of the polygon touch the circle - each line corresponds to the energy level of the MOs at those atoms

A dashed horizontal line half way up the circle indicates the separation of bonding and antibonding orbitals

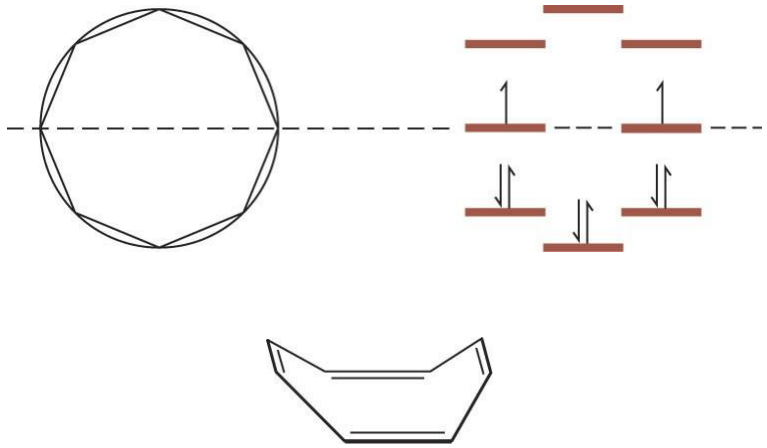
➔ **Benzene has 3 bonding and 3 antibonding orbitals**

All the bonding orbitals are full and there are no electrons in antibonding orbitals; benzene has a closed shell of delocalized electrons and is very stable



➔ **Cyclooctatetraene has two nonbonding orbitals each with one electron**

This is an unstable configuration; cyclooctatetraene adopts a nonplanar conformation with localized π bonds to avoid this instability



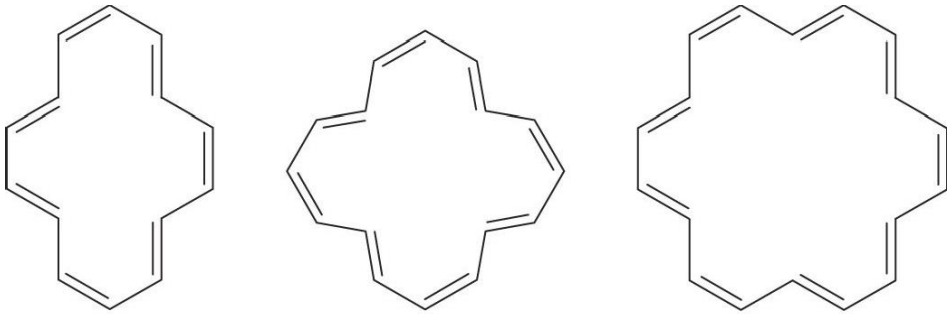
– The Annulenes

➔ Annulenes are monocyclic compounds with alternating double and single bonds

Annulenes are named using a number in brackets that indicates the ring size
Benzene is [6]annulene and cyclooctatetraene is [8]annulene
An annulene is aromatic if it has 4n+2π electrons and a planar carbon skeleton

➔ The [14]and [18]annulenes are aromatic (4n+2, where n= 3,4)

The [16] annulene is not aromatic

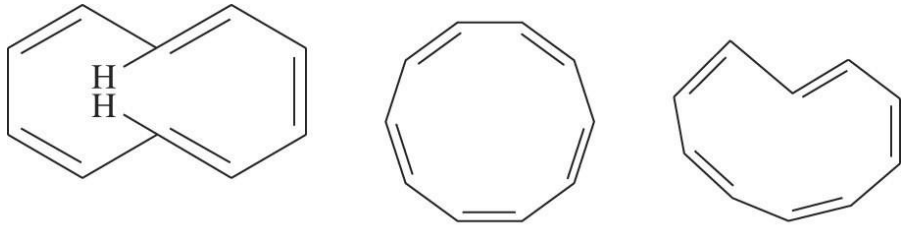


[14]Annulene (aromatic) **[16]Annulene (*not* aromatic)** **[18]Annulene (aromatic)**

➔ **The [10] annulenes below should be aromatic but none of themcan be planar**

4 is not planar because of steric interaction of the indicated hydrogens

5 and 6 are not be planar because of large angle strain in the flat molecules



4 **5** **6**

[10]Annulenes

None is aromatic because none is planar.

➔Cyclobutadiene is a [4]annulene and is not aromatic

It does not follow the 4n+ 2 rule and is highly unstable

Cyclobutadiene
or [4]annulene
(*not* aromatic)