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Study Notes on Aromaticity

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Aromaticity

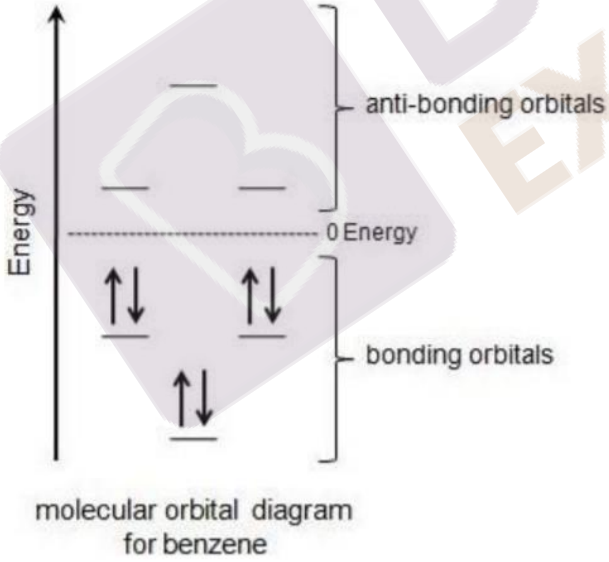
Aromaticity can be defined as a property of conjugated cycloalkenes which helps in enhancing the stabilization of the molecule .This happens because of the delocalization of π electrons.

The **Hückel's rule** for aromaticity are:

1. Molecule is cyclic
2. Every atom of the ring must have one p orbital
3. Molecule should be planar and every atom must have a sp^2 hybridized orbital
4. Molecule must have 4n+2 pi-bond electrons, where n is equal to any integer (0,1,2,3,…)

According to **Hückel's Molecular Orbital Theory**, a compound is stable if all the bonding molecular orbitals are completely filled with a pair of electrons. No anti-bonding orbital should be occupied.

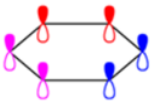
Benzene has 6 π electrons. The first 2 π electrons fill up the lowest energy orbital, and the remaining 4 π electrons get filled in the succeeding energy level. In this manner ,all its bonding orbitals are filled, but none of the anti-bonding orbitals have any electrons. Therefore, the molecule shows exceptional stability



molecular orbital diagram for benzene

Aromatic compounds are highly stable compounds. On the other hand, Anti-aromatic compounds have an unusual instability. They have similar rules to aromaticity except the fact that the molecule has a closed loop of 4n pi-bond electrons.

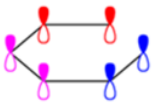
benzene



1. Cyclic
2. *p*-orbital for each member of the ring
3. Planar ring (sp^2 hybridized)
4. **4n+2 π–bond electron count.**

Aromatic

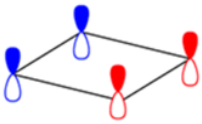
hexatriene



1. NOT Cyclic
2. *p*-orbital for each member of the ring
3. Planar ring (sp^2 hybridized)
4. **4n+2 π–bond electron count.**

Non-Aromatic

cyclobutadiene



1. Cyclic
2. *p*-orbital for each member of the ring
3. Planar ring (sp^2 hybridized)
4. **Closed 4n π–bond electron count.**

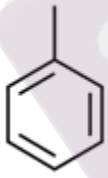
Anti-Aromatic

Benzenoid and Non-benzenoid compounds

Benzenoid compounds:

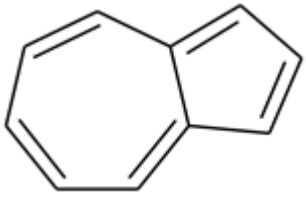
These molecules contain at least one benzene ring in their structure.A benzene ring has a cyclic structure and has six carbon atoms.It has a conjugated pi system containing alternate double and single bonds.

Since the molecule has double bonds because of the presence of a benzene ring, the molecule shows extra stability provided by the conjugated pi system. For example: toluene



Non-benzenoid compounds:

These molecules exhibit an aromatic behaviour without having any benzene nucleus . They have one or more rings fused but none of the rings is a benzene ring . The ring structure of these compounds might contain 5-7 etc number of carbons. The most common example is AZULENE . It is a system of two fused rings , one containing 7 and the other 5 carbons.



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