3.3. Aromaticity

3.3.1. Condition for aromaticity

- The structure should be cyclic,
- The cyclic structure has to be planner,
- Total number of π-electrons in the molecule or ion must be (4n+2) where n = 0,1,2,3….
- Each of the atoms in the cyclic structure should be sp^2-hybridized, having on e unhybridized π-orbital,
- The unhybridized p-orbitals overlap to form a continuous ring of parallel orbitals,
- The delocalization of π-electrons over the ring decreases the electronic energy.

3.3.2. Huckel rule

This rule states that a planner conjugated monocyclic polyene having (4n+2)π-electrons where n = 0, 1, 2, 3, 4…… shows aromatic character and the molecule will be highly stable.

3.3.3. General rules for a molecule to be aromatic, anti-aromatic and non-aromatic

❖ For aromaticity please follow section 3.3.1.

➢ Anti-aromaticity: Planner conjugated monocyclic polyenes in which π-electron delocalization increases electronic energy (destabilization) are anti-aromatic system.

➢ The essential requirement of aromaticity and anti-aromaticity is the overlap of parallel p-orbitals.

▪ For non-aromatic system, the system will be cyclic but not planner that means the parallel p-orbital overlap is unavailable.

3.3.4. Aromaticity of Annulenes

Conjugated monocyclic polyenes having structural formula CnHn are usually called annulenes. The reported annulenes have n = 12. 14, 16, 18, 20, 24 and 30, out of those only [14], [18], [30] annulenes are (4n+2)π-electron molecules. The rest of the molecules are (4n) electronic system.

3.3.5. Influence of electron density on aromaticity

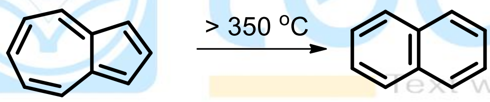
When a lone pair of electron on an atom in the aromatic ring is utilized to gain aromaticity, then the lone pair is not readily available for donation to other species. e.g. pyrrole is weak base, because the lone pair of electron on N atom of the pyrrole ring is a part of six delocalized π-electrons. So, the compound will be weak base. However, if the lone pair is donated, then it will no longer be aromatic and hence it will be unstable.

3.3.6. Aromaticity and stability of fullerences

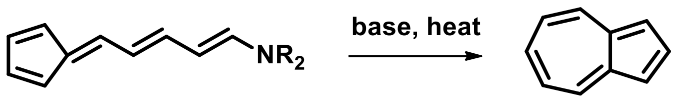
- Fullerenes are cage like structure.
- It has geometry of a truncated icosahedron or geodesic dome.
- The geometry of C_{60} is icosahedron with sixty vertices, one carbon at each.
- There are 32 faces, 12 of which are pentagons and 20 of which are hexagon.
- Each pentagon is surrounded by five hexagons.
- No two pentagons are adjacent.

3.3.7. Azulene

- It is deep blue compound
- It is isomeric with naphthalene and its stability is less than naphthalene.
- It is non-benzenoid aromatic compound.



- It is prepared from fulvene.

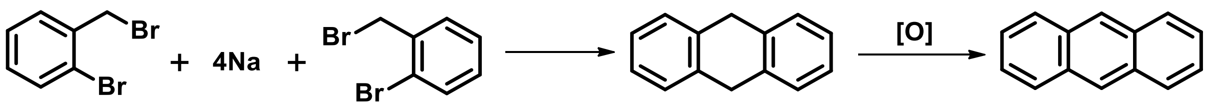


3.3.8. Polycyclic aromatic compounds

Common examples of polycyclic aromatic compounds are naphthalene, phenanthrene, and pyrene.

Preparation:

3.3.8a. Fittig reaction:



3.3.8b. Elbs reaction: