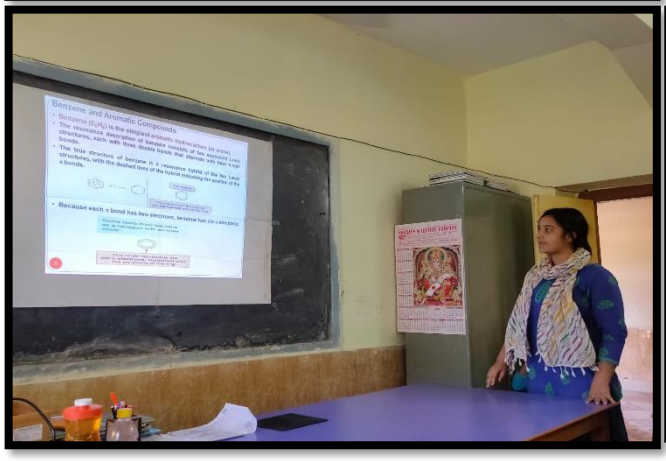
Departmental Student Seminar organized by Department of Chemistry

Date: 23rd November, 2021

Departmental student seminar was organised by Chemistry Department on 23rd N 2021. All the students from Chemistry Department have presented PowerPoint pr on the topic from current chemistry research under the guidance of our faculty me

No. of teachers present: 04
No. of students present: 10

Snapshot of the Seminar



Student Seminar Presentation

Structure & Functional Properties of Aromatic Compounds

Manidipa Singha Mahapatra

1st Semester

Department of Chemistry

KHATRA ADIBASI MAHAVIDYALAYA

Khatra: Bankura: West Bengal

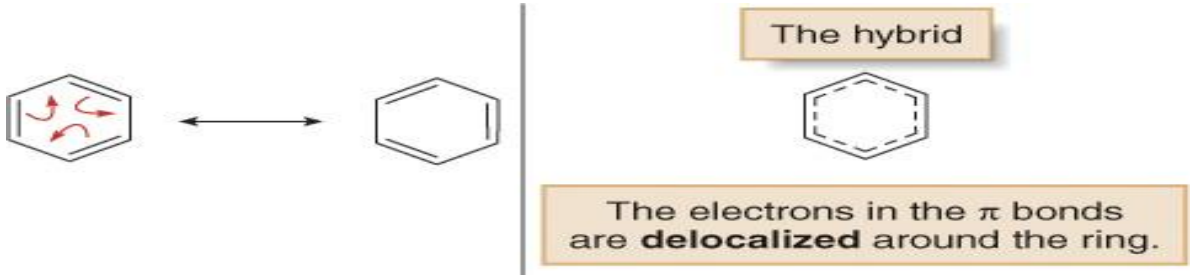
Date: 23rd November 2021

Contain

- Benzene and Aromatic Compounds
- Nomenclature of Benzene Derivatives
- Stability of Benzene
- The Criteria for Aromaticity—Hückel's Rule
- Examples of Aromatic Rings

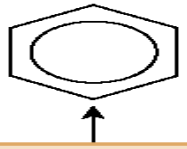
Benzene and Aromatic Compounds

- **Benzene (C_6H_6) is the simplest aromatic hydrocarbon (or arene).**
- **The resonance description of benzene consists of two equivalent Lewis structures, each with three double bonds that alternate with three single bonds.**
- **The true structure of benzene is a resonance hybrid of the two Lewis structures, with the dashed lines of the hybrid indicating the position of the π bonds.**



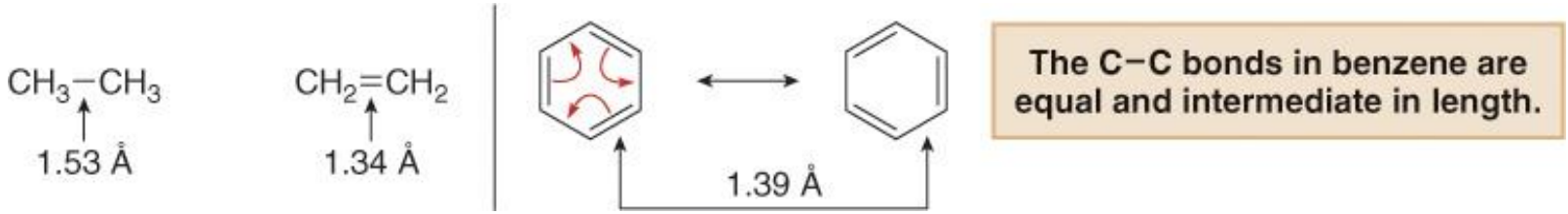
- **Because each π bond has two electrons, benzene has six π electrons.**

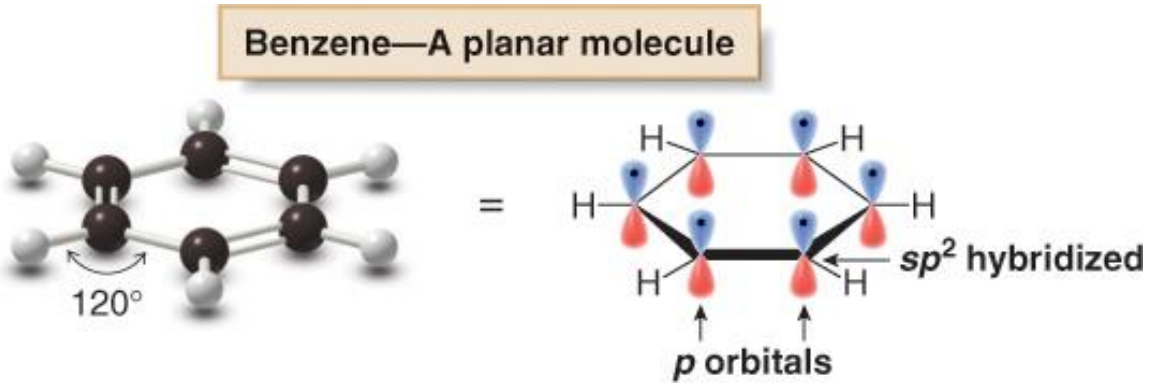
Some texts draw benzene as a hexagon with an inner circle:



The circle represents the **six π electrons,** distributed over the six atoms of the ring.

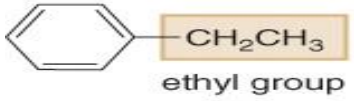
- **In benzene, the actual bond length (1.39 Å) is intermediate between the carbon—carbon single bond (1.53 Å) and the carbon—carbon double bond (1.34 Å).**



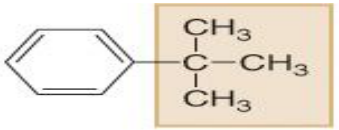


Nomenclature of Benzene Derivatives

- **To name a benzene ring with one substituent, name the substituent and add the word benzene.**



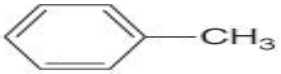
ethylbenzene



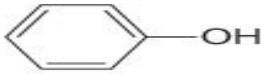
tert-butylbenzene

chlorobenzene

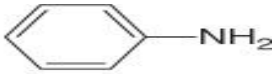
- **Many monosubstituted benzenes have common names which you must also learn.**



toluene
(methylbenzene)



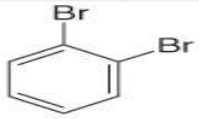
phenol
(hydroxybenzene)



aniline
(aminobenzene)

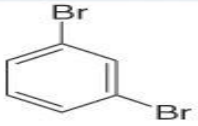
- **There are three different ways that two groups can be attached to a benzene ring, so a prefix—ortho, meta, or para—can be used to designate the relative position of the two substituents.**

1,2-disubstituted benzene
ortho isomer



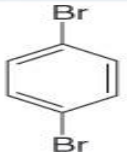
***ortho*-dibromobenzene**
or
***o*-dibromobenzene**
or 1,2-dibromobenzene

1,3-disubstituted benzene
meta isomer



***meta*-dibromobenzene**
or
***m*-dibromobenzene**
or 1,3-dibromobenzene

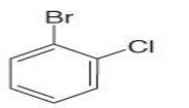
1,4-disubstituted benzene
para isomer



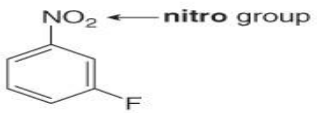
***para*-dibromobenzene**
or
***p*-dibromobenzene**
or 1,4-dibromobenzene

- **If the two groups on the benzene ring are different, alphabetize the names of the substituent preceding the word benzene.**
- **If one substituent is part of a common root, name the molecule as a derivative of that monosubstituted benzene.**

Alphabetize two different substituent names:

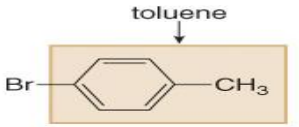


***o*-bromochloro-benzene**

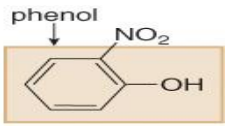


***m*-fluoronitro-benzene**

Use a common root name:

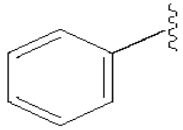


***p*-bromo**toluene



***o*-nitro**phenol

- **A benzene substituent is called a phenyl group, and it can be abbreviated in a structure as "Ph-".**

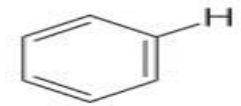


abbreviated as **Ph—**

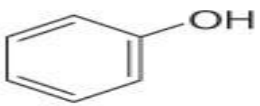
phenyl group
C_6H_5—

- A phenyl group (C_6H_5—) is formed by removing one hydrogen from benzene (C_6H_6).

- **Therefore, benzene can be represented as PhH, and phenol would be PhOH.**

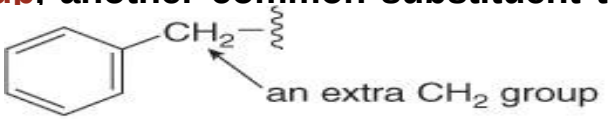


benzene = **C_6H_5—H**
PhH

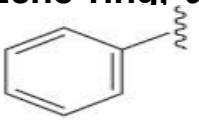


phenol = **C_6H_5—OH**
PhOH

- **The benzyl group, another common substituent that contains a benzene ring, differs from a phenyl group.**



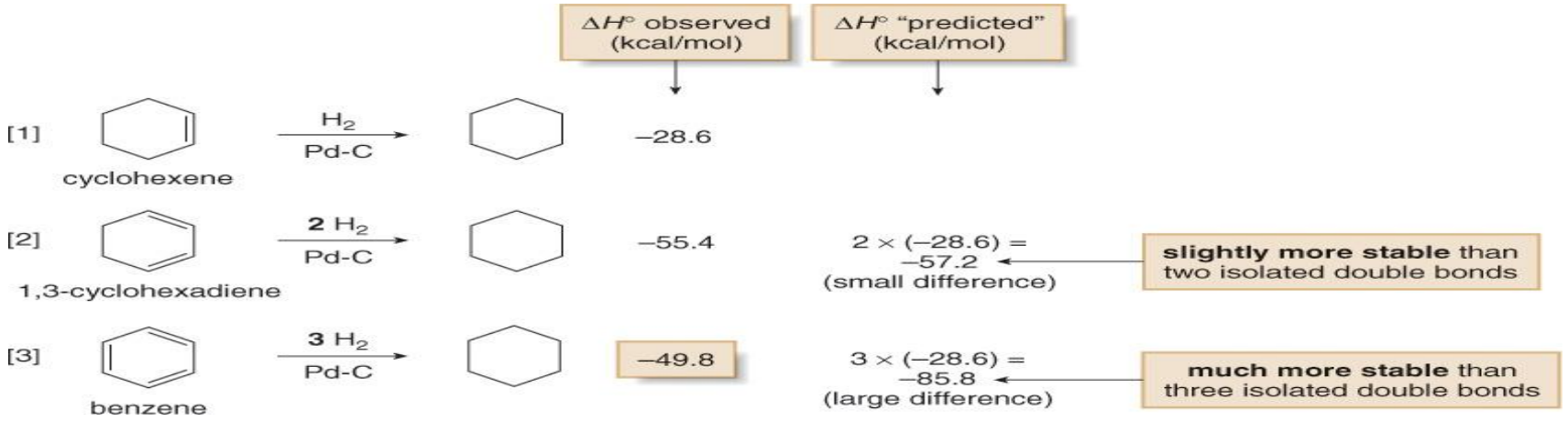
benzyl group
$C_6H_5CH_2$—



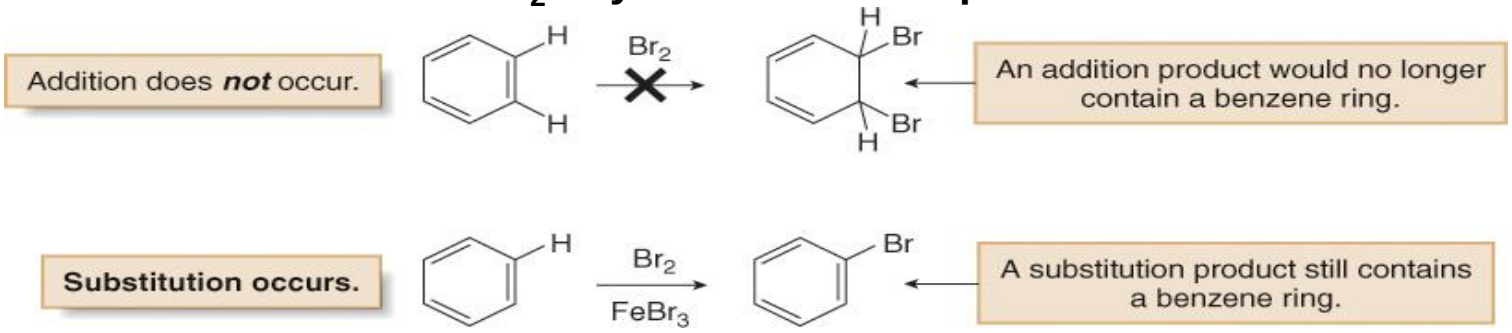
phenyl group
C_6H_5—

Stability of Benzene

- **Consider the heats of hydrogenation of cyclohexene, 1,3-cyclohexadiene and benzene, all of which give cyclohexane when treated with excess hydrogen in the presence of a metal catalyst.**



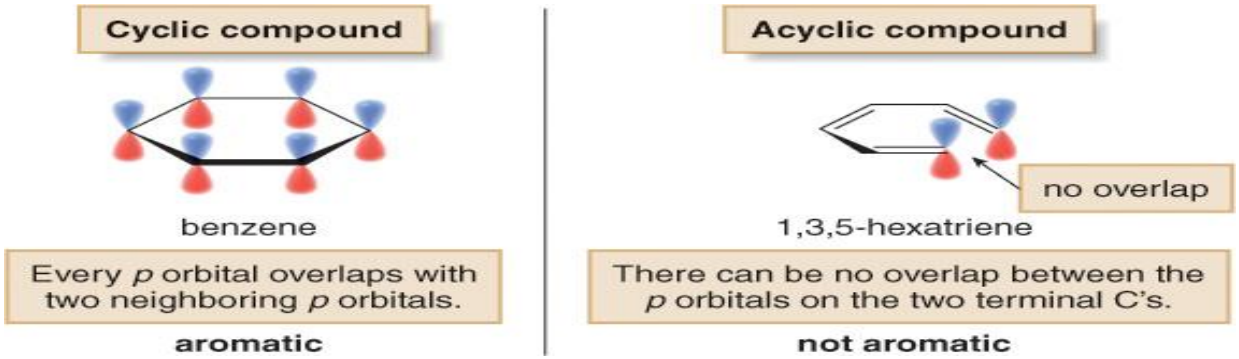
- **The low heat of hydrogenation of benzene means that benzene is especially stable. This unusual stability is characteristic of aromatic compounds.**
- **Benzene's unusual behavior is not limited to hydrogenation. Benzene does not undergo addition reactions.**
- **Benzene does not react with Br_2 to yield an addition product.**



The Criteria for Aromaticity—Hückel's Rule

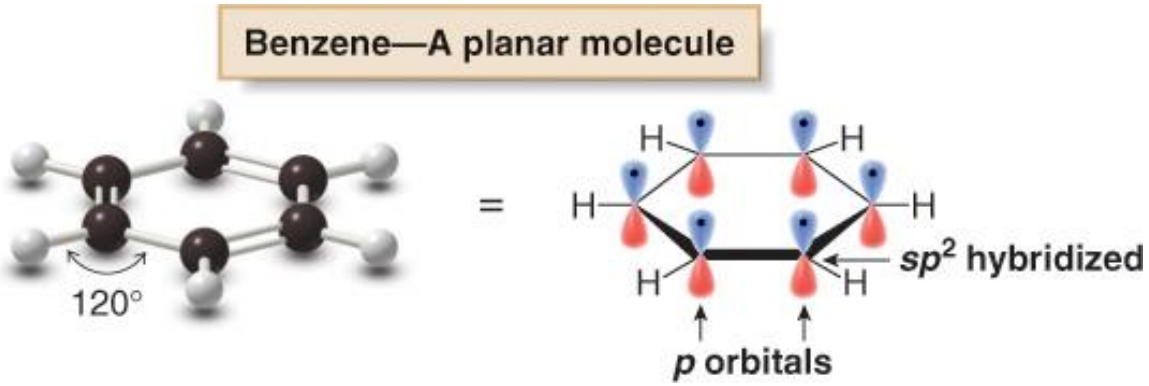
Four structural criteria must be satisfied for a compound to be aromatic.

[1] A molecule must be cyclic.



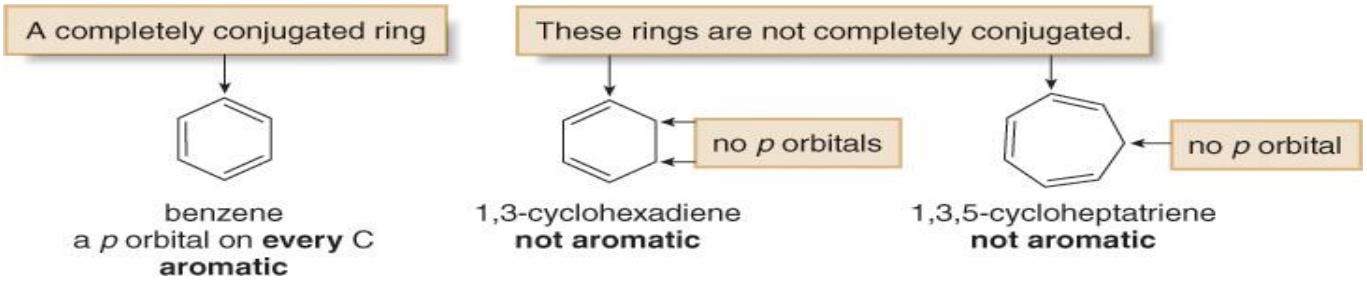
To be aromatic, each *p* orbital must overlap with *p* orbitals on adjacent atoms.

[2] A molecule must be planar.



[3] A molecule must be completely conjugated.

Aromatic compounds must have a *p* orbital on every atom.

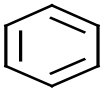


[4] A molecule must satisfy Hückel's rule, and contain a particular number of π electrons.

Hückel's rule:

An aromatic compound must contain 4n+2π electrons [n (integer no.) = 0, 1, 2, and so…]

Benzene is aromatic and especially stable because it contains 6 π electrons. Cyclobutadiene is nonaromatic and especially unstable because it contains 4 π electrons.

Benzene	Cyclobutadiene
An aromatic compound	non-aromatic compound
	
4n+2= 6 π e	4n+2=4 π e
4n=6 - 2=4	4n= 4 - 2 =2
n=4/4=1	n=2/4 = 1.5
aromatic	non-aromatic

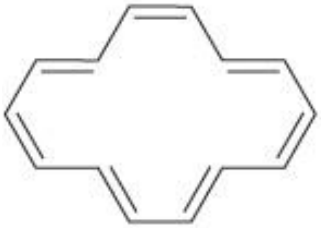
Note that Hückel's rule refers to the number of π electrons, not the number of atoms in a particular ring.

Table 17.2 The Number of π Electrons That Satisfy Hückel's Rule

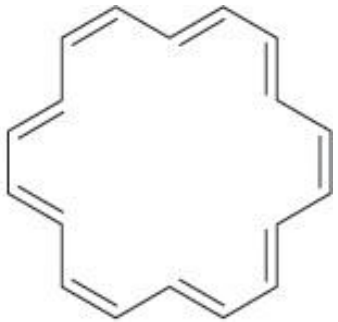
n	4*n* + 2
0	2
1	6
2	10
3	14
4, etc.	18

Examples of Aromatic Rings

- **Completely conjugated rings larger than benzene are also aromatic if they are planar and have $4n + 2$ π electrons.**
- **Hydrocarbons containing a single ring with alternating double and single bonds are called annulenes.**
- **To name an annulene, indicate the number of atoms in the ring in brackets and add the word annulene.**



[14]-annulene
$4n + 2 = 4(3) + 2 =$
14 π electrons
aromatic



[18]-annulene
$4n + 2 = 4(4) + 2 =$
18 π electrons
aromatic

- **Thus, although five resonance structures can also be drawn for the cyclopentadienyl cation and radical, only the cyclopentadienyl anion has 6 π electrons, a number that satisfies Hückel's rule.**

cyclopentadienyl anion
- **6** π electrons
- contains $4n + 2$ π electrons

aromatic

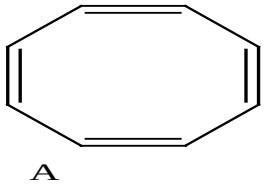
cyclopentadienyl cation
- **4** π electrons
- contains $4n$ π electrons

antiaromatic

cyclopentadienyl radical
- **5** π electrons
- does not contain either $4n$ or $4n + 2$ π electrons

nonaromatic

Indicate which of the following are aromatic and non-aromatic?



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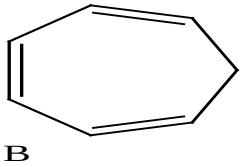

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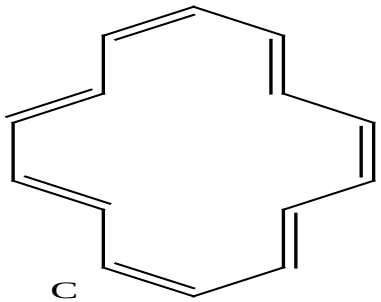
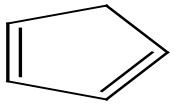


C



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