

12.3 AROMATIC COMPOUNDS

Introduction to aromatic Compounds

- In earlier time, compounds are called **aromatic** because of their **pleasant odours**.



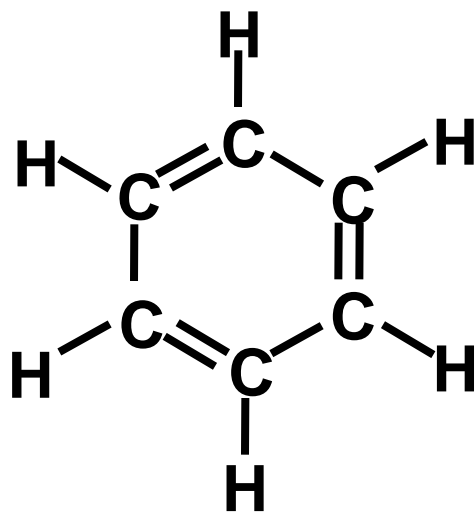
Benzene has strong pleasant odour.

- Today, we use the word **aromatic** to refer to **benzene** and its **structural relatives**.

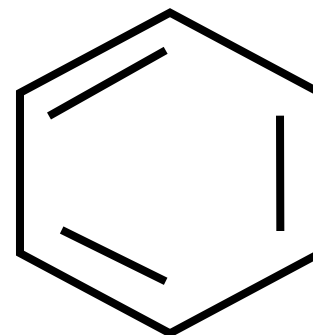
- **Aromatic compound is a cyclic conjugated molecule or ion that is stabilized by π electron delocalisation.**
- **It is characterised by substitution reactions.**

KEKULÉ'S STRUCTURE

- Kekule was the first to formulate a reasonable representation of benzene



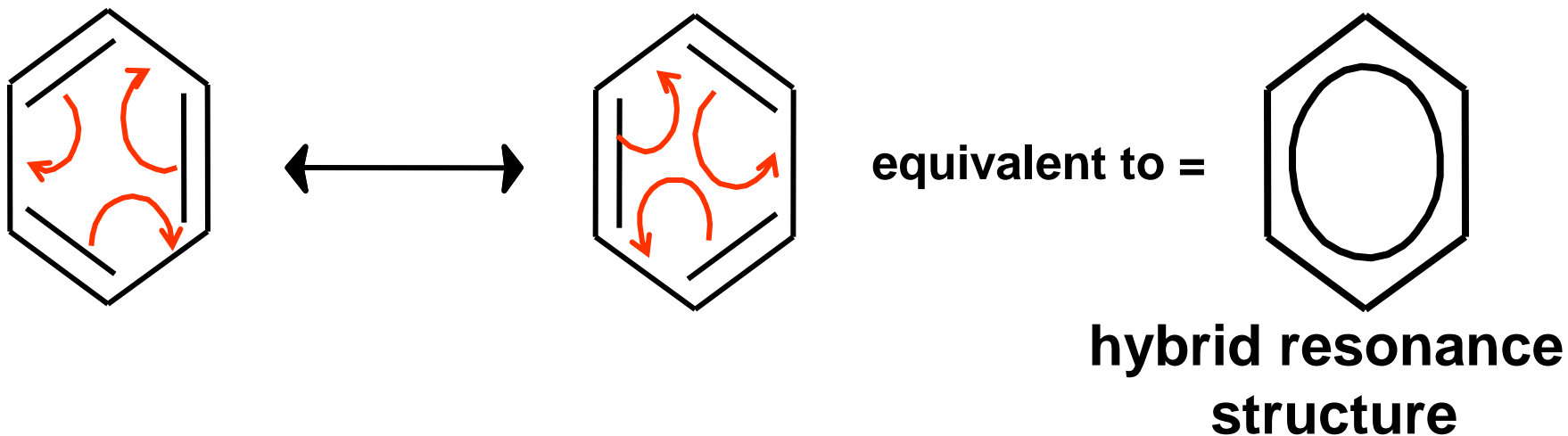
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The Kekule structure suggests alternating double and single carbon-carbon bonds

RESONANCE STRUCTURE

- Benzene is actually a **resonance hybrid** of the **two Kekulé structures**.



- All **C–C bond length equal** = 139 pm
- Shorter than typical C–C (148 pm)
- Longer than typical C=C (134 pm)

THE CRITERIA FOR AROMATICITY

■ 4 structural criteria must be satisfied for compound to be aromatic

Cyclic

Planar

Completely conjugated

Contain particular number of π electron
❖ obeys Hückel's Rule



THE CRITERIA FOR AROMATICITY

Hückel's Rule



Erich Hückel
(1896-1980)

* cyclic, planar and completely conjugated compounds that contain $[4n+2]$ π electron ($n=0,1,2,\dots$) are said to be aromatic

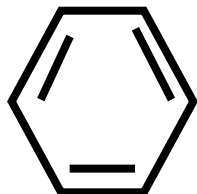
❖ planar monocyclic rings with 2,6,10,14 and so forth π electrons are aromatic

THE CRITERIA FOR AROMATICITY

EXAMPLE OF AROMATIC COMPOUNDS

1. Aromatic compounds with a single ring

Benzene



aromatic

Benzene is aromatic because:

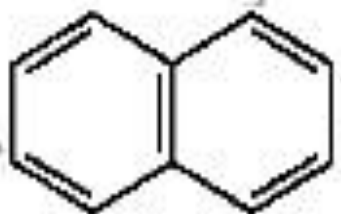
- contains 6π electrons (obeys Hückel's Rule)
- cyclic, planar and has double bond in the ring

$$\begin{aligned} [4n+2] \pi &= [4(1) + 2]\pi \\ &= 6 \pi \text{ electrons} \end{aligned}$$

THE CRITERIA FOR AROMATICITY

2. Aromatic compounds with more than one ring

EXAMPLE



naphthalene

$$4n+2 = 4(2) + 2$$

10 π electrons

Aromatic

* Two benzene rings joined together forms naphthalene

DISCOVERY OF BENZENE

- Benzene is a colourless, volatile, highly flammable, non-polar liquid, with a characteristic aromatic odour. Its physical properties include:

Molecular weight	78.11
Density	0.88 gcm ⁻³
Melting point	20°C
Boiling point	80.1°C
Solubility	Slightly soluble in water Very soluble in organic solvents and oil

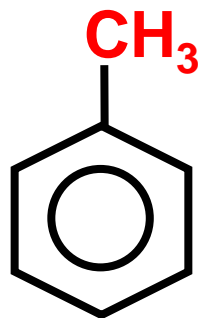
NAMING BENZENE & ITS DERIVATIVES

- Many organic molecules contain a **benzene ring** with one or more **substituents**.



Many **common name** are **recognized** by the **IUPAC system**

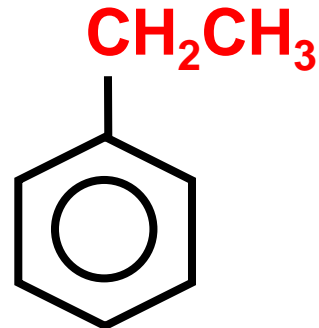
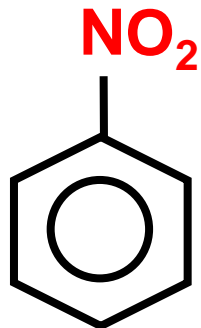
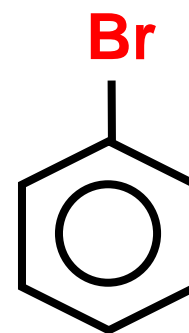
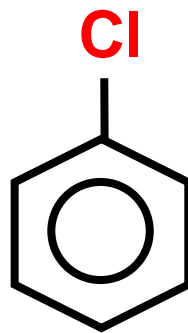
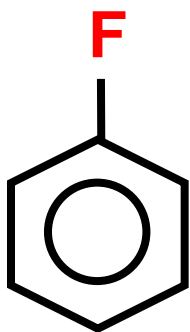
EXAMPLE:



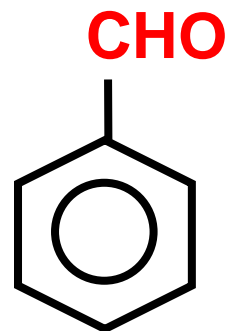
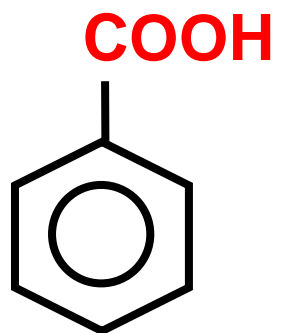
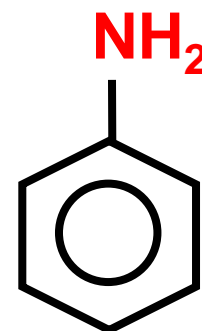
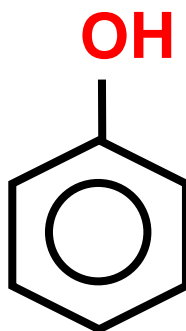
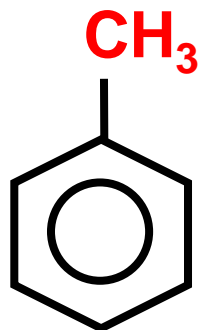
Common: **toluene**
IUPAC: **methylbenzene**

MONO SUBSTITUTED BENZENE

- **Benzene** is the **parent name** and the **substituent** is indicated by a **prefix**.



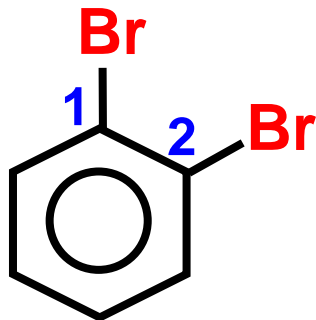
- **IUPAC** rules **allow** some **common names** to be retained.



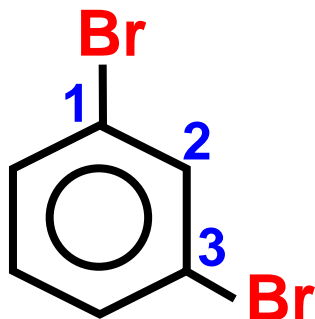
DISUBSTITUTED BENZENE

Two Same Substituents

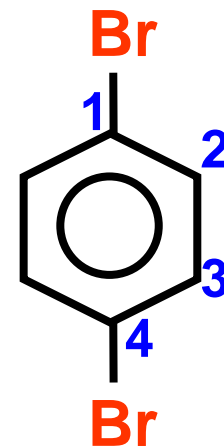
- Relative position of substituents are indicated by prefixes *ortho*, *meta*, and *para* (*o-*, *m-*, and *p-*) or by the use of **number**.



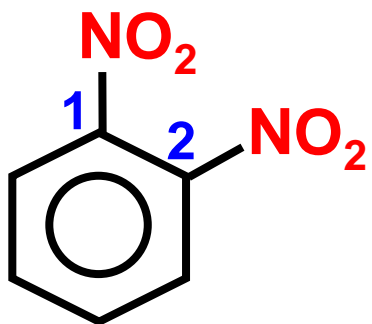
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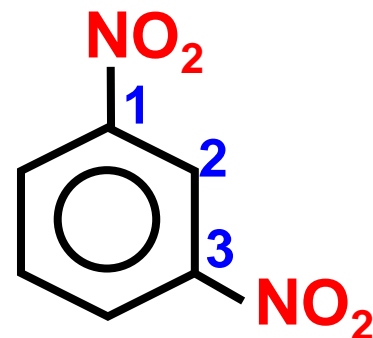
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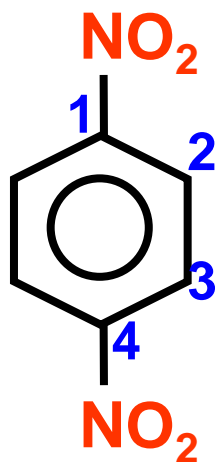
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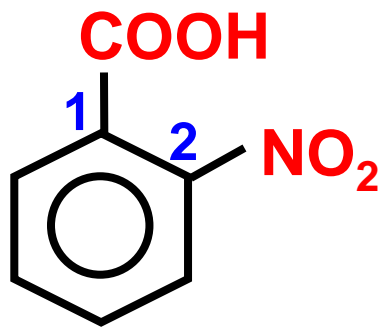
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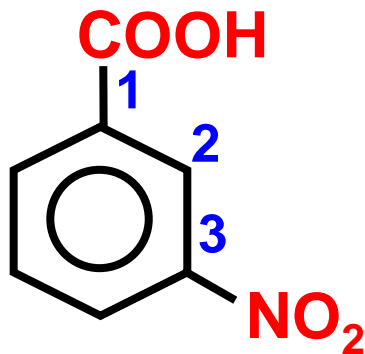
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Two Different Substituents

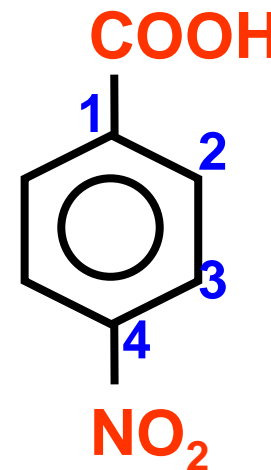
- Select **one** of the **substituent** that give **new parent name** and numbered as **C1**.



or



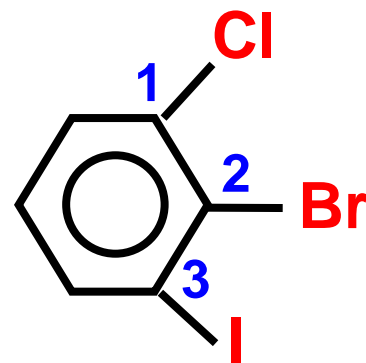
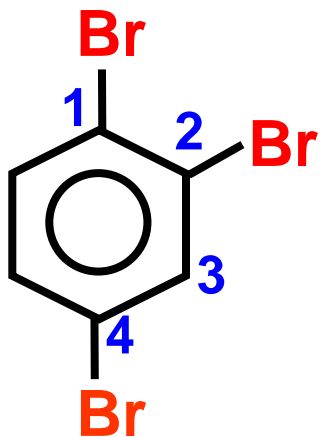
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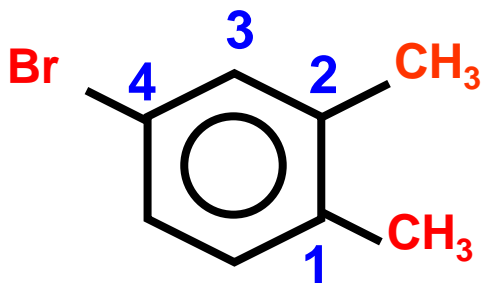
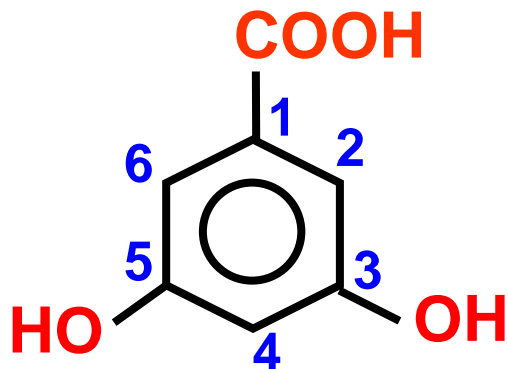
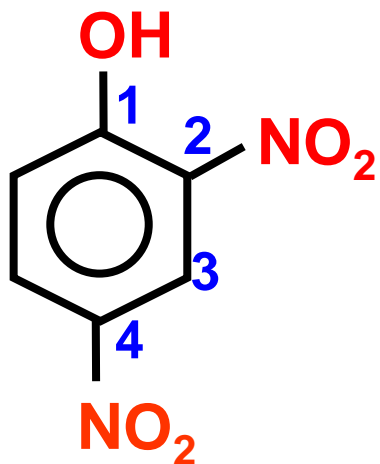
or

THREE OR MORE SUBSTITUENTS

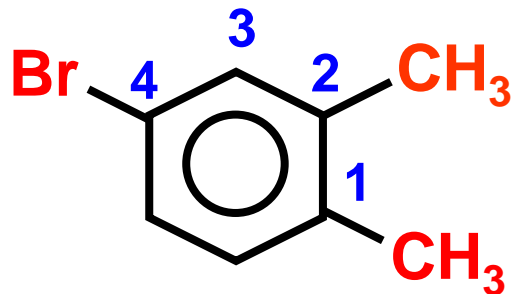
- Position of substituents must be indicated by **numbers**.
- The substituents are listed **alphabetically** when writing the name.



- C atom bearing the substituent that define the new parent name is numbered as **C1**.



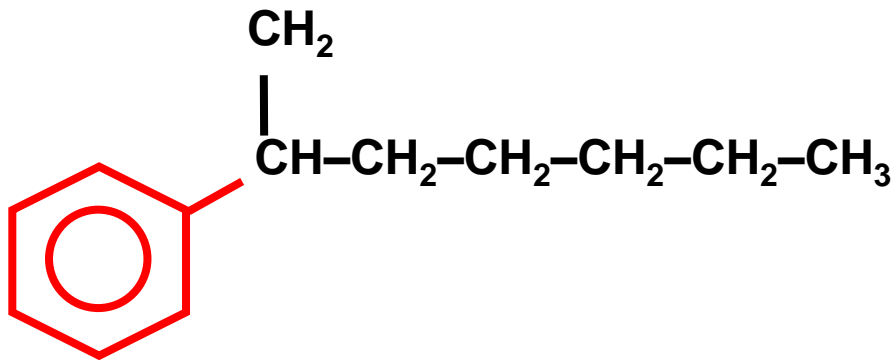
Keep in mind!



o-, *m*- and *p*- naming system is used for arenes with **2 substituents only!**

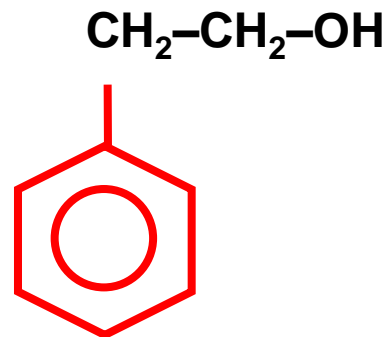
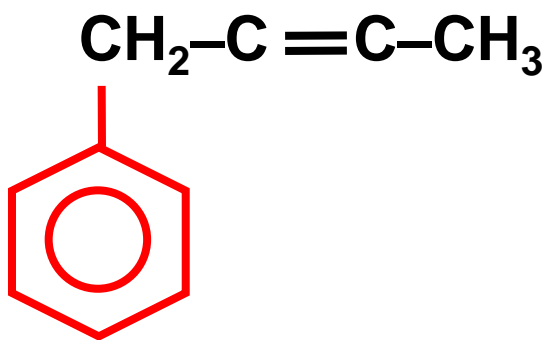
PHENYL GROUP

- **Benzene ring as substituent.**
- **If alkyl substituent is larger than the ring (more than 6 C), the compound is named as **phenyl-substituted alkane.****

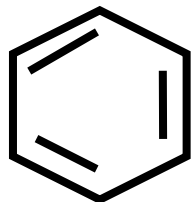


- **Phenyl = C₆H₅- = Ph**

- If the chain is **unsaturated** (have **C=C** or **C≡C**) or contains **important functional group**, the **benzene ring** is considered as **phenyl substituent**.

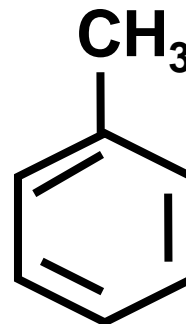


CARCINOGENIC EFFECT



benzene

replaced by



toluene



- Many aromatic compounds are **carcinogenic** and **toxic**.
- Example: **benzene**, **benzo[a]pyrene**.

- At one time, benzene was widely used as **solvent**.
 - Studies revealed benzene is **carcinogenic** (can cause **cancer**).
 - Replaced by **toluene**.
-

- **Benzo[a]pyrene** is found in **cigarette smoke, automobile exhaust**, and the fumes from **charcoal grills**.
-

- When ingested or inhaled, it oxidised to **carcinogenic products**.
-

- **Benzoic acid** **organic acid** **prevent growth many organism**
-

- Widely used as a food preservative.

The end....

