

# AQA Chemistry A-Level

## 3.3.10: Aromatic Chemistry

### Detailed Notes

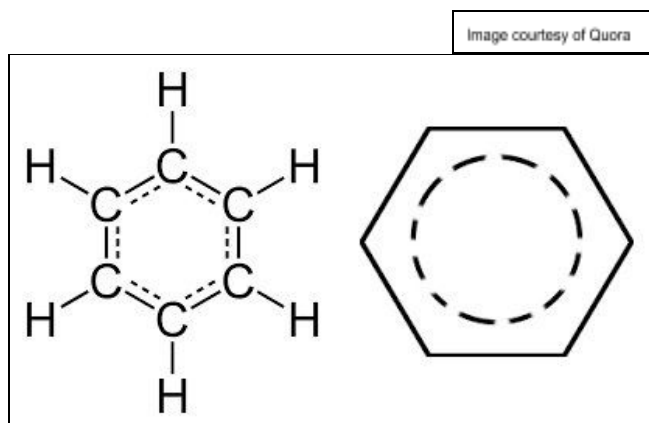




### 3.3.10.1 - Bonding

Benzene is an **aromatic compound** consisting of a ring of **six carbon atoms** with **six hydrogen atoms** and a ring of **delocalised electrons**:

*Example:*



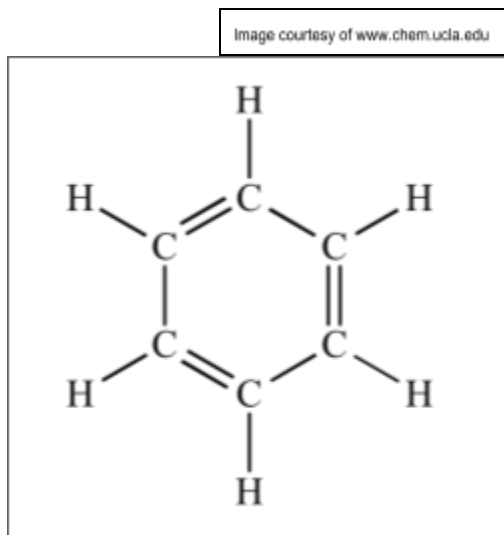
Each bond in the benzene ring has an **intermediate length** in between that of a double and single bond.

The outer electron from the **p-orbital** of each carbon atom is **delocalised** to form the central ring. This ring structure makes benzene **very stable** compared to other molecules of a similar size.

#### Cyclohexatriene vs. Benzene

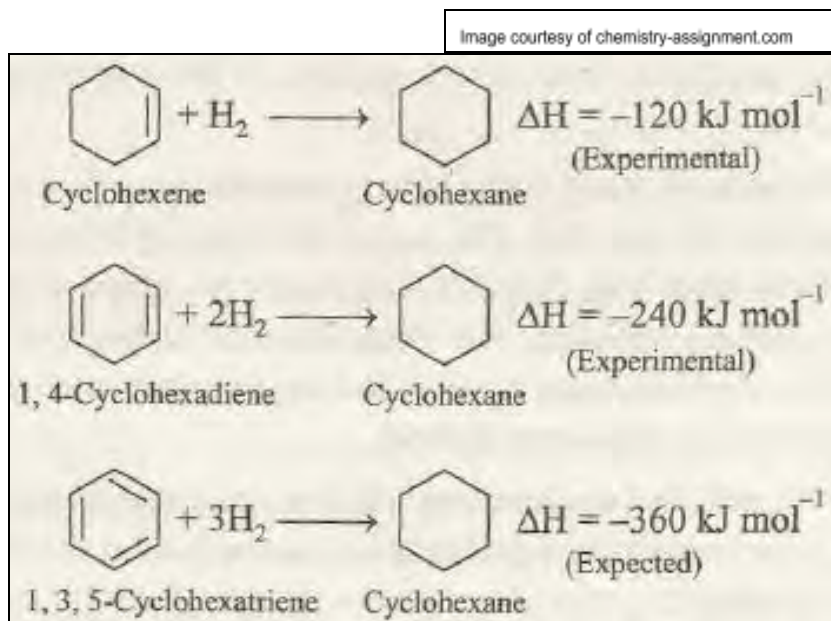
When benzene was first discovered its structure was not known. It was predicted from empirical measurements that it had the structure similar to that of **cyclohexatriene**, with three double bonds and three single bonds.

*Example:*



Therefore the enthalpy change of hydrogenation for benzene was **predicted to be  $-360\text{kJmol}^{-1}$** , three times the enthalpy change of cyclohexene.

*Example:*



It was later discovered that the enthalpy change of hydrogenation of benzene was **actually  $-208\text{kJmol}^{-1}$**  leading to the conclusion of its **different, unusual structure**.

### Arenes

Compounds that **contain benzene as part of their structure** are called arenes or aromatic compounds. They have **high melting points** due to the high stability of the delocalised ring, but **low boiling points** as they are **non-polar** molecules and **cannot often be dissolved** in water.

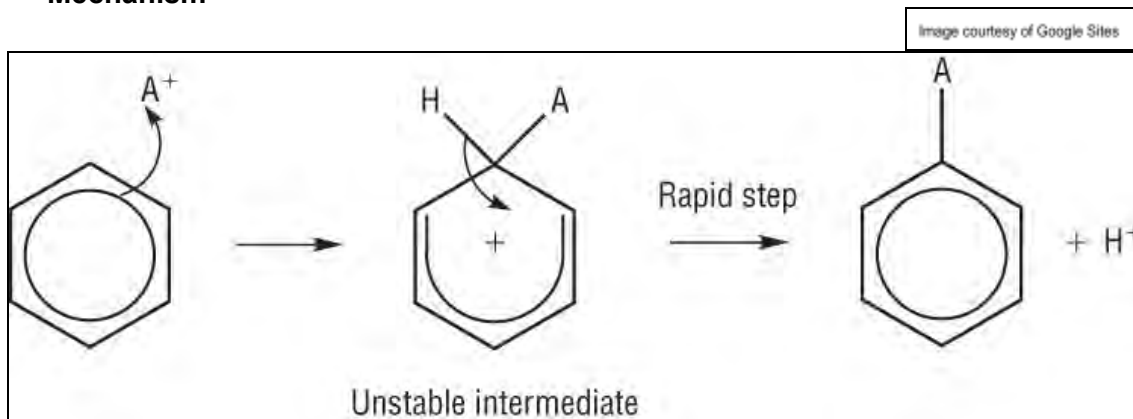
### 3.3.10.2 - Electrophilic Substitution

The delocalised ring in benzene is an **area of high electron density** making it susceptible to attack from **electrophiles**. When these species attack the electron ring, it is **partially destroyed** then **restored** in the process of **electrophilic substitution**. This mechanism means aromatic amines and nitrobenzene can be produced from benzene.





### Mechanism

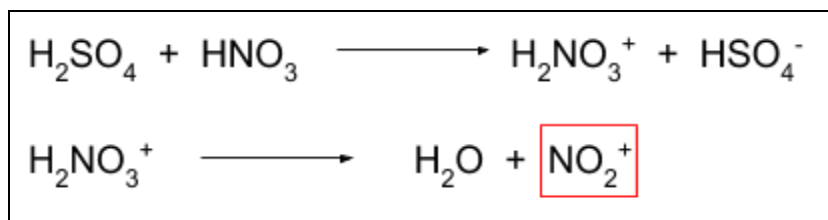


*The nucleophile is shown as  $A^+$ .*

### Nitrobenzene

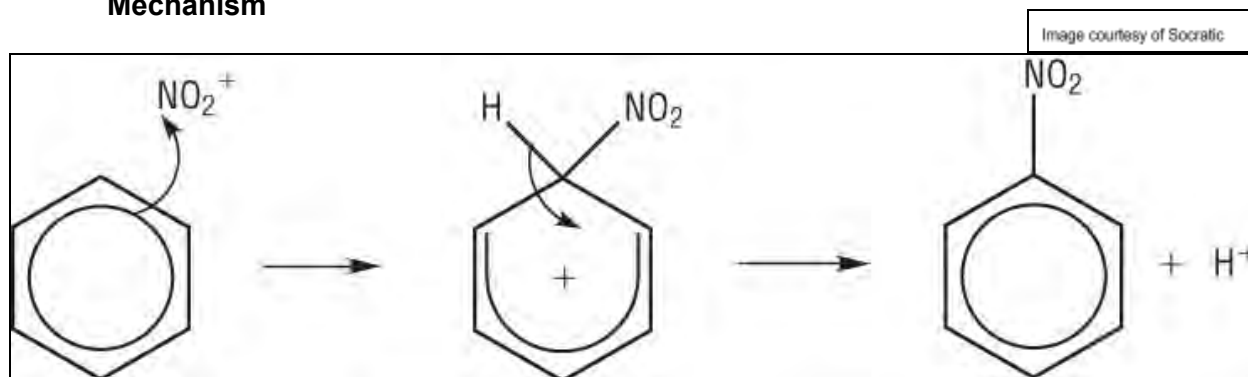
In this form of electrophilic addition, the electrophile is the  $\text{NO}_2^+$  ion. This is a **reactive intermediate**, produced in the reaction of concentrated sulfuric acid ( $\text{H}_2\text{SO}_4$ ) with concentrated nitric acid ( $\text{HNO}_3$ ).

Example:



When heated with benzene these reagents lead to the **substitution of the  $\text{NO}_2^+$  electrophile** onto the benzene ring, **removing a hydrogen** ion.

### Mechanism



This reaction shows a **mono-substitution** of a single  $\text{NO}_2^+$  electrophile which takes places when the reaction temperature is  **$55^\circ\text{C}$** . At temperatures greater than this, multiple substitutions can occur. It is vital that only one substitution occurs for the production of **aromatic amines**.



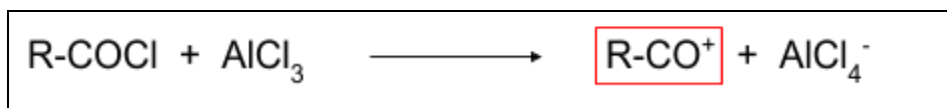


## Friedel-Crafts Acylation

The delocalised electron ring in benzene can also act as a **nucleophile**, leading to the **attack on acyl chlorides**. This reaction is known as **Friedel-Crafts acylation**.

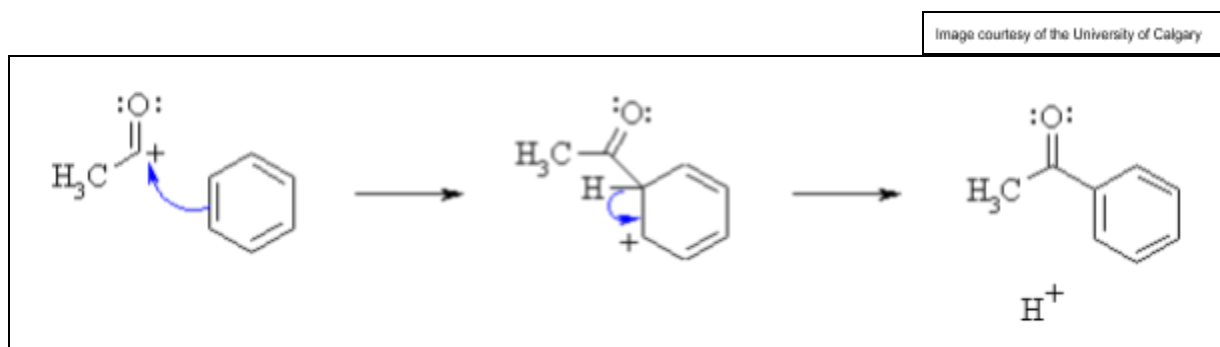
In order for it to take place, a **reactive intermediate** must be produced from the acyl chloride and an **aluminium chloride catalyst**.

*Example:*



This reactive intermediate is then attacked by the benzene ring.

### Mechanism



At the end of the reaction, the  $\text{H}^+$  ion removed from the ring reacts with the  $\text{AlCl}_4^-$  ion to reform the aluminium chloride, showing it to be a **catalyst**.

The product of this reaction is a **phenylketone**. In this case, the benzene group is called a **phenyl group**. These molecules are commonly used in the industrial production of dyes, pharmaceuticals and even explosives.

