Reactions of Benzene

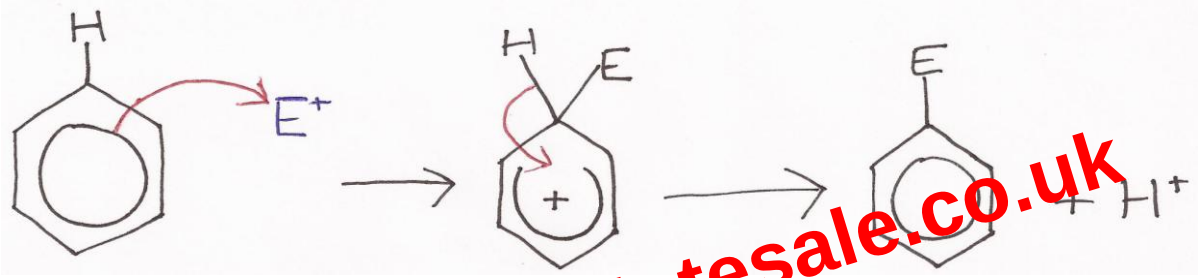
Benzene undergoes reduction reactions as one of the six hydrogen atoms is subsitituted by the reacting functional group.

The delocalised electron is a region of high electron density so generally involve reaction with electron deficient chemical species which accept electrons to form new covalent bonds.

Electrophilic Substitution

1. Electrophile E^+ is attracted to the delocalised electron cloud of the benzene ring structure
2. Electrophile bonds to the benzene ring via two of the six delocalised electrons, leaving a partially delocalised system containing four delocalised electrons. This temporarily causes the loss of natural stability of the six electron delocalised system.
3. H^+ is lost by breaking the C-H bond. Electrons from this bond re- form the stable delocalised six electron system

Mechanism

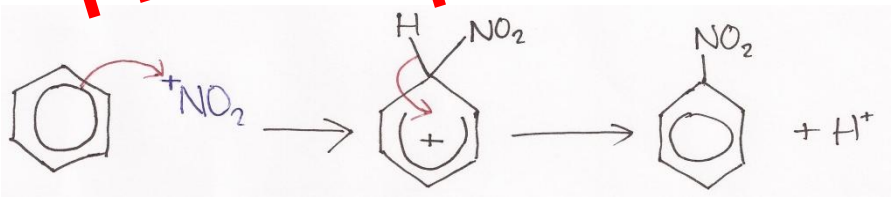


The reaction conditions are generally severe;

- Heat
- Concentrated reagents and catalysts to make these reactions take place

This is because of the high stability of the delocalised benzene structure

Electrophiles generated easily are; NO_2^+, Nitro group and $CH3C^+O$, Acyl group



Nitration of Benzene via Electrophilic Subsitution

Conditions/ Reagents; Concentrated sulphuric acid, H_2SO_4 and concentrated nitric acid, HNO_3 at 50°c

The nitric acid provides the nitro group. The sulphuric acid donates a proton to the nitric acid.

$C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$

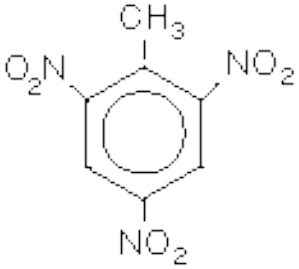
Step one- Formation of the electrophile $^+NO_2$

Overall; $2H_2SO_4 + HNO_3 \rightarrow {}^+NO_2 + H_3O^+ + 2HSO_4^-$

By $H_2SO_4 + HNO_3 \rightarrow HSO_4^- + H_2NO_3$

$H_2NO_3 \rightarrow {}^+NO_2 + H_2O$

$H_2O + H_2SO_4 \rightarrow H_3O^+ + HSO_4^-$



Trinitrotoluene (TNT)

Nitrobenzenes can be used as explosives e.g. TNT (Trinitrotoluene)