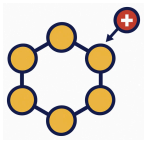
Substitution and Phenol Map

Edexcel A Level Chemistry · Topic 18A Electrophilic Substitution and Phenol

1 The mechanism

18A.5

- π-electrons attack E^+
- Horseshoe intermediate, + inside
- C–H breaks: **H^+ lost**
- Delocalisation **restored**



2 Nitration

18A.4, 18A.5

- Conc HNO_3 + conc H_2SO_4
- **Below 55 °C**
- Electrophile **NO_2^+**
- Hotter: 1,3-dinitrobenzene

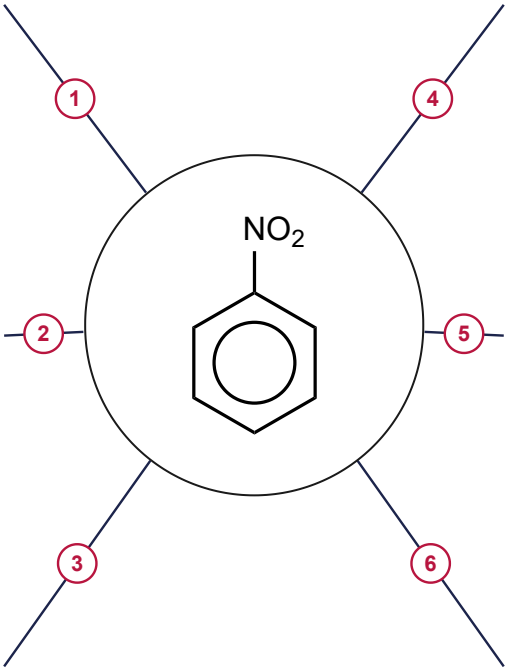


3 Halogenation

18A.4, 18A.5

- Halogen carrier: $FeBr_3$, Fe, $AlBr_3$
- $Br_2 + FeBr_3 \rightarrow Br^+ + FeBr_4^-$
- Product bromobenzene + HBr
- Carrier is **regenerated**

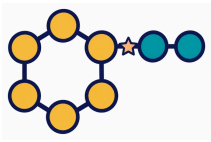




4 Friedel-Crafts

18A.4, 18A.5

- Anhydrous **$AlCl_3$**, reflux
- RCl gives R^+: alkylation
- RCOCl gives RCO^+: acylation
- New **C–C bond** to the ring



5 Combustion

18A.4

- High C:H: **smoky flame**
- Soot is unburnt carbon
- $7½O_2$ for complete burning
- Benzene is **92% carbon**



6 Phenol

18A.6, 18A.7

- O lone pair joins the π-system
- Higher density **polarises Br_2**
- No carrier: white precipitate
- 2,4,6-tribromophenol



Electrophiles

how each one forms, and the catalyst that returns

Reaction	Electrophile	Forming it	Catalyst back
Nitration	NO_2^+	$HNO_3 + H_2SO_4$	$H^+ + HSO_4^- \rightarrow H_2SO_4$
Bromination	Br^+	$Br_2 + FeBr_3$	$H^+ + FeBr_4^- \rightarrow FeBr_3 + HBr$
Chlorination	Cl^+	$Cl_2 + AlCl_3$	$H^+ + AlCl_4^- \rightarrow AlCl_3 + HCl$
Alkylation	$CH_3CH_2^+$	$CH_3CH_2Cl + AlCl_3$	$H^+ + AlCl_4^- \rightarrow AlCl_3 + HCl$
Acylation	CH_3CO^+	$CH_3COCl + AlCl_3$	$H^+ + AlCl_4^- \rightarrow AlCl_3 + HCl$

Worked examples

Yield

- 7.8 g C_6H_6: 0.100 mol
- 8.61 g product: 0.0700 mol
- **70%**

Phenol

- 0.940 g: 0.0100 mol
- Mr of product 331
- **3.31 g**

Combustion

- 0.200 mol benzene
- × 7½
- **1.50 mol O_2**

Nitrobenzene is reduced to phenylamine in the amines section of Topic 18.

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