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20.2 Synthetic Routes

IB Chemistry - Revision Notes

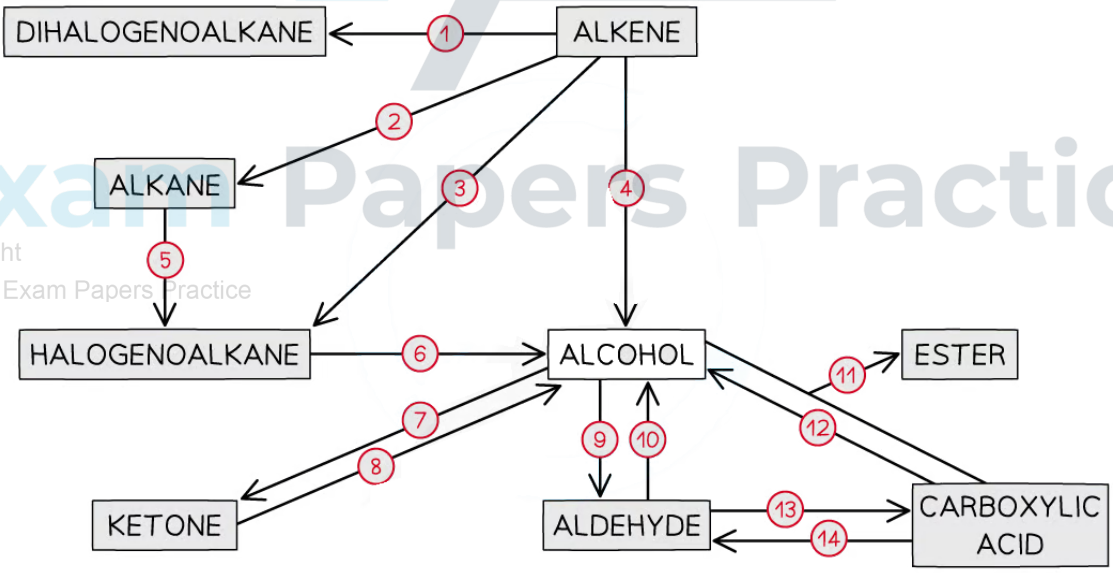
20.2.1 Synthesis

Organic Synthesis

- It is possible to make a large number of organic products from a few starting compounds and the necessary reagents and conditions
- Knowing how organic functional groups are related to each other is key to the synthesis of a given molecule
- The main functional groups you need to know are
  - Alkanes
  - Alkenes
  - Halogenoalkanes
  - Alcohols
  - Carbonyls (aldehydes & ketones)
  - Carboxylic acids and derivatives
  - Arenes

Aliphatic Reaction Pathways

- The key functional groups and their interconversions are summarised here:



The main reaction pathways in aliphatic chemistry

Aliphatic Chemistry Reactions Table

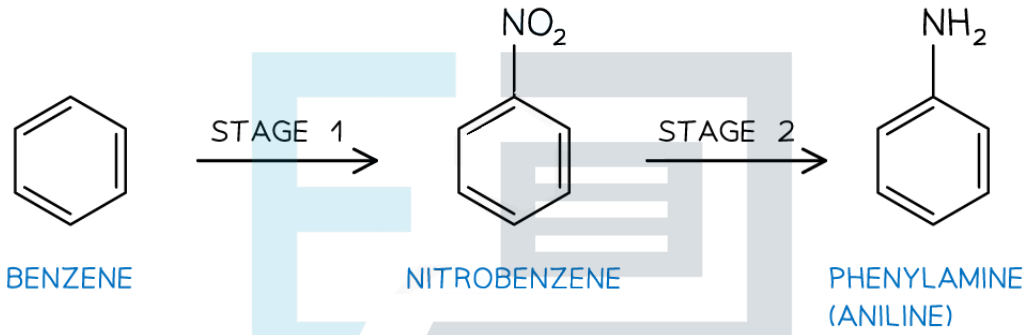
Reaction	Reagent(s)	Conditions	Mechanism	Reaction type
1	Halogen	Room temperature	Electrophilic	Addition
2	Hydrogen	Ni catalyst 200°C / 1000 kPa	Electrophilic	Addition / Reduction
3	Hydrogen halide	Room temperature	Electrophilic	Addition
4	Steam + H_2SO_4	Heat	–	Hydration
5	Halogen	UV light	Free radical	Substitution
6	NaOH (aq)	Heat under reflux	Nucleophilic	Substitution
7	$K_2Cr_2O_7$ / H_2SO_4	Heat	–	Oxidation
8	$NaBH_4$ (aq)	Heat	–	Reduction
9	$K_2Cr_2O_7$ / H_2SO_4	Heat	–	Oxidation
10	$NaBH_4$ (aq)	Heat	–	Reduction
11	Alcohol + carboxylic acid, H_2SO_4 catalyst	Heat	–	Esterification / condensation
12	$LiAlH_4$ in dry ether	Heat	–	Reduction
13	$K_2Cr_2O_7$ / H_2SO_4	Heat under reflux	–	Oxidation
14	$LiAlH_4$ in dry ether	Heat	–	Reduction

Exam Tip

Remember, that due to the strength of the $LiAlH_4$ as a reducing agent, it is unlikely that reaction 14 can be stopped at the aldehyde To form an aldehyde from a carboxylic acid, you reduce the carboxylic acid to a primary alcohol and then oxidise it to the aldehyde

Aromatic Reaction Pathways

- The key aromatic reaction for this course is:



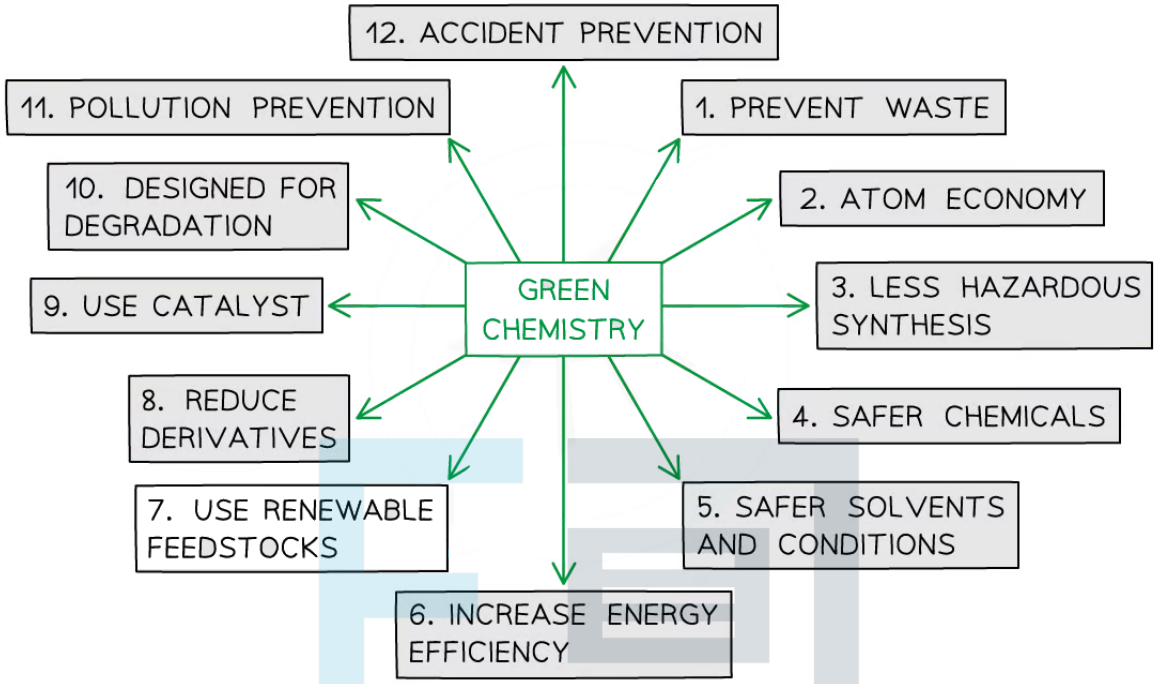
The nitration and reduction reactions to form phenylamine from benzene

Aromatic Nitration and Reduction Reactions Table

Reaction	Reagent	Conditions	Mechanism	Reaction type
1	Conc. NHO_3 + H_2SO_4	25–60℃	Electrophilic	Substitution
2	Sn + Conc HCl followed by NaOH (aq)	Heat	–	Reduction

Choosing A Reaction Pathway

- Chemists will often have several choices of reaching a target molecule and those choices need to take into the principles of green chemistry



The twelve principles of green chemistry

- By choosing a pathway that has fewer steps, you can prevent waste and reduce energy demands which is better for the environment
  - This also reduces production costs
- By analysing the atom economy of each step, you can select reactions that give a higher atom economy
- Choosing alternative safer solvents also follows the principles of green chemistry

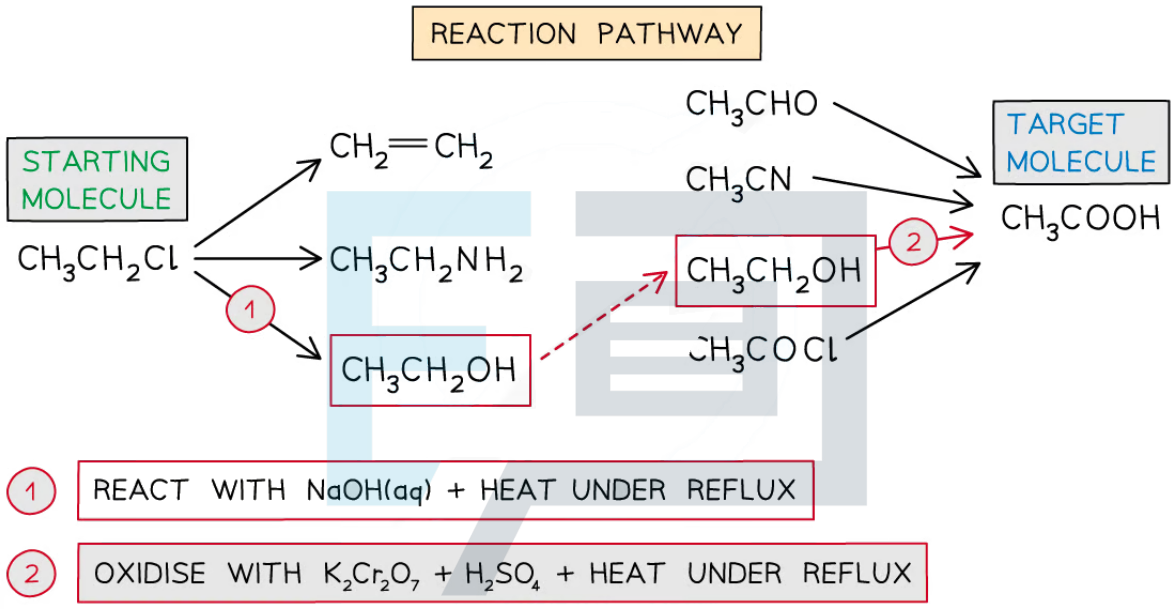
Designing a Reaction Pathway

- The given molecule is usually called the **target molecule** and chemists try to design a synthesis as efficiently as possible
- Designing a reaction pathway starts by drawing the structures of the target molecule and the **starting molecule**
- Work out all the compounds that can be made from the starting molecule and all the molecules that can be made into the target molecule
  - Match the groups they have in common and work out the reagents and conditions needed

Worked example

Suggest how the synthesis of ethanoic acid from chloroethane could be carried out

Answer



Exam Tip

You could be required to design a synthesis with up to four steps.