Edexcel organic reaction mechanisms

Click a box below to go to the mechanism

Click here for advice

Homolytic

Free Radical Substitution

Free Radical Addition

Heterolytic

Electrophilic Addition

Nucleophilic Substitution | S_N2 | S_N1

Electrophilic Substitution | Nitration | Br_2 | Alkylation | Acylation

Nucleophilic Addition

Free radical substitution

chlorination of methane

i.e. homolytic breaking of covalent bonds

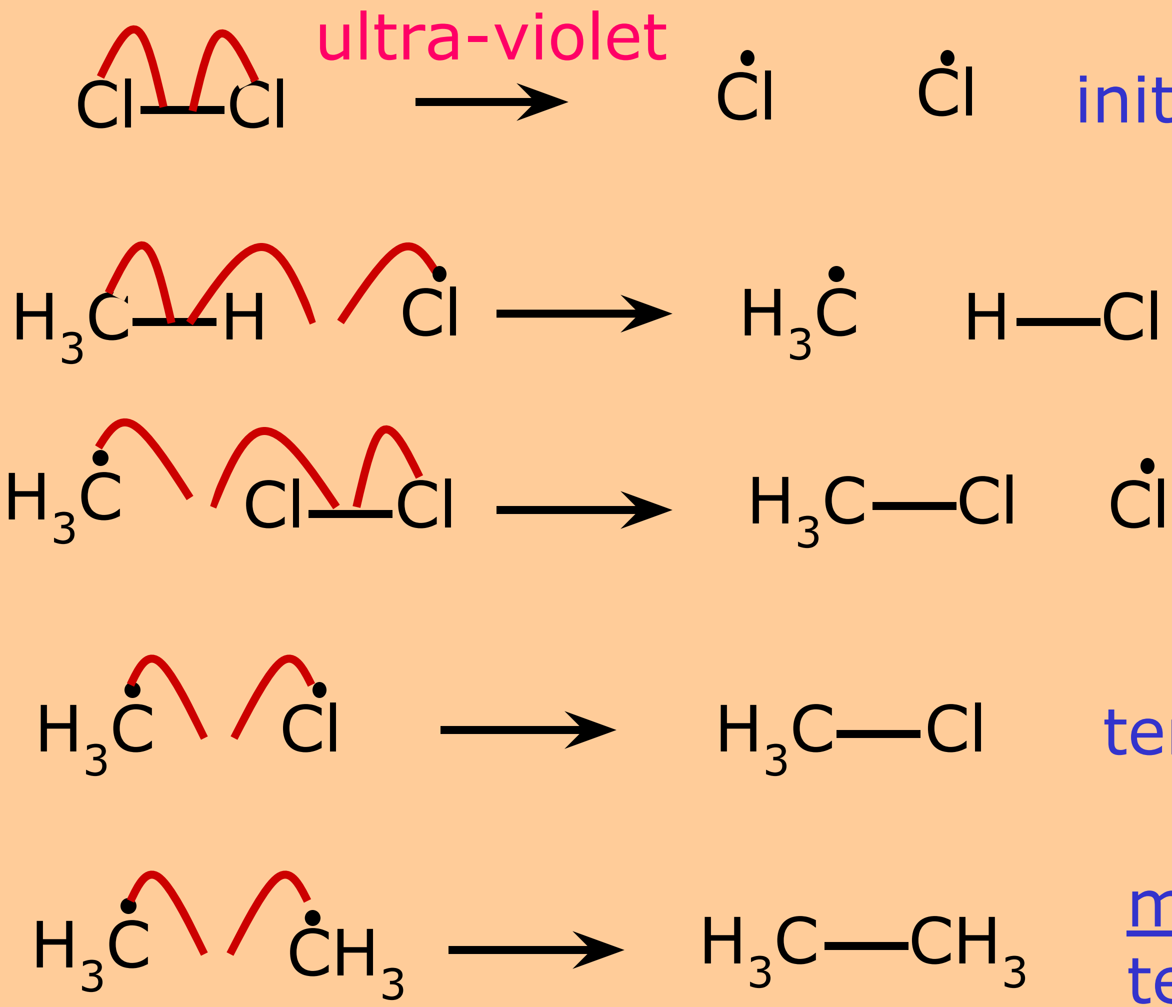
Overall reaction equation

$$CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$$

Conditions

ultra violet light
excess methane to reduce further substitution

Free radical substitution mechanism



initiation step

two propagation steps

termination step

minor termination step

Further free radical substitutions

Overall reaction equations

$$CH_3Cl + Cl_2 \longrightarrow CH_2Cl_2 + HCl$$

$$CH_2Cl_2 + Cl_2 \longrightarrow CHCl_3 + HCl$$

$$CHCl_3 + Cl_2 \longrightarrow CCl_4 + HCl$$

Conditions ultra-violet light
excess chlorine

Free radical addition

addition polymerisation of ethene

i.e. homolytic breaking of covalent bonds

Overall reaction equation

$$n\ H_2C{=}CH_2 \longrightarrow -\!\!\left[CH_2CH_2\right]\!\!-_n$$

ethene → polyethene

Conditions

free radical source
(a species that generates free radicals
that allow the polymerisation of ethene molecules)

Free radical addition mechanism

$$R\text{—}R \longrightarrow \dot{R} \quad \dot{R}$$

initiation step

$$H_2C{=}CH_2 \quad \dot{R} \longrightarrow H_2\dot{C}\text{—}CH_2\text{—}R$$

$$H_2C{=}CH_2 \quad H_2\dot{C}\text{—}CH_2R \longrightarrow H_2\dot{C}\text{—}CH_2\text{—}CH_2CH_2R$$

chain propagation steps

Addition of $H_2C{=}CH_2$ repeats the same way until:

$$R(CH_2)_n\dot{C}H_2 \quad H_2\dot{C}(CH_2)_mR \longrightarrow R(CH_2)_nCH_2\text{—}CH_2(CH_2)_mR$$

termination step

polyethene

Electrophilic addition

bromine with propene

mechanism

$$CH_3CH{=}CH_2 + Br_2 \longrightarrow CH_3CHBrCH_2Br$$

1,2-dibromopropane

hydrogen bromide with but-2-ene

mechanism

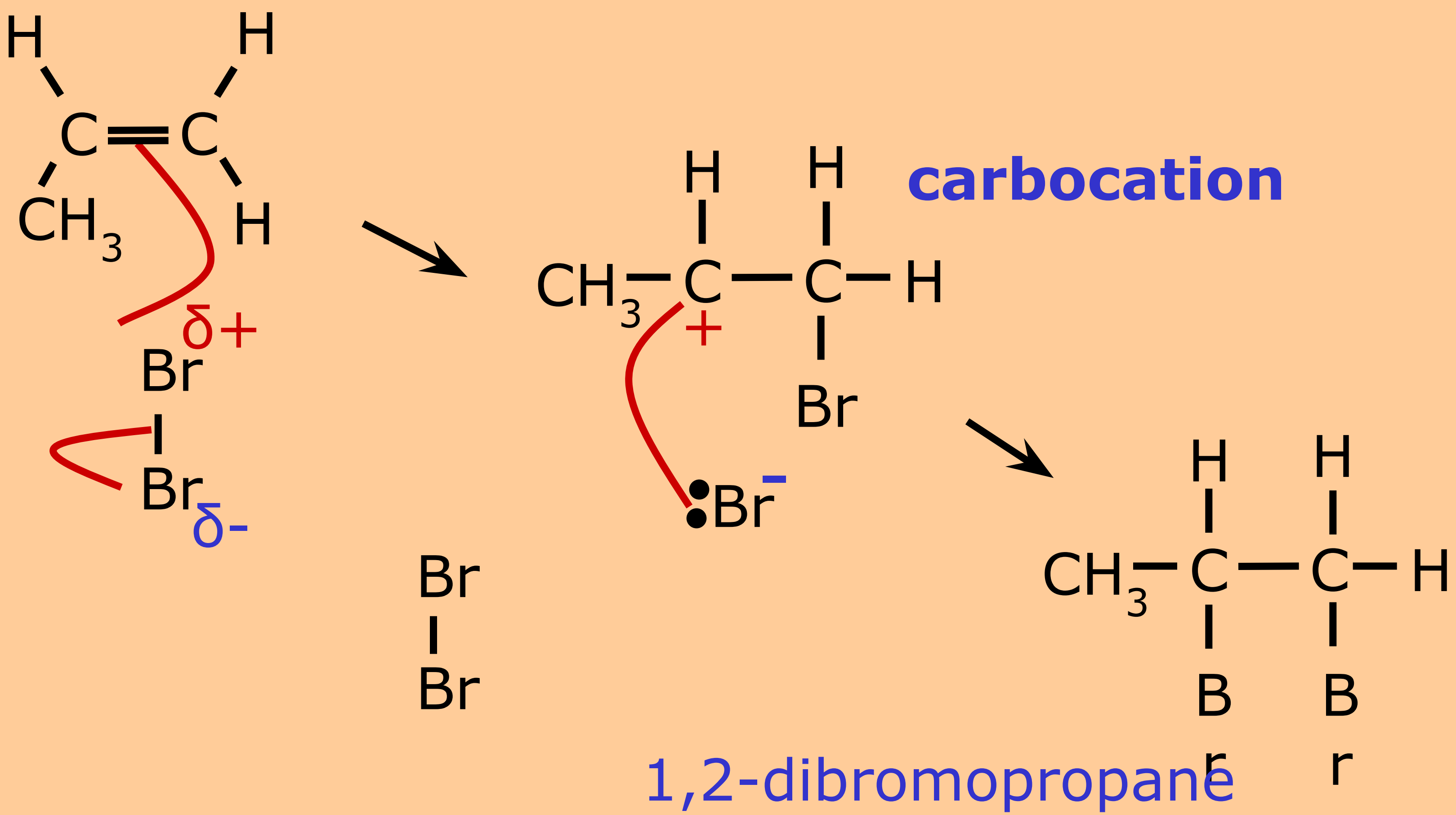
$$CH_3CH{=}CHCH_3 + HBr \longrightarrow CH_3CH_2CHBrCH_3$$

2-bromobutane

Electrophilic addition mechanism

bromine with propene

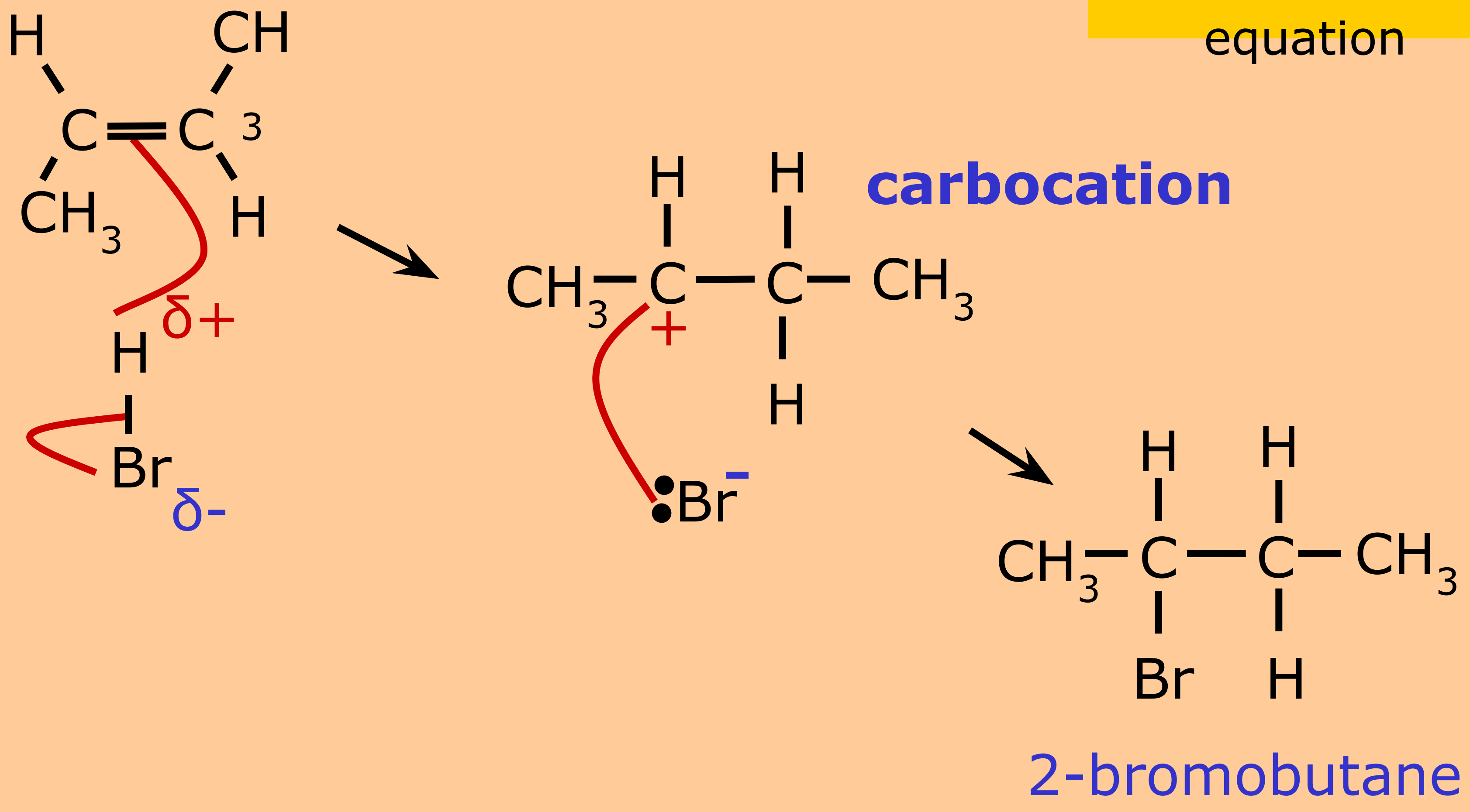
reaction equation



Electrophilic addition mechanism

hydrogen bromide with trans but-2-ene

reaction equation



Original slide prepared for the RS•C

Nucleophilic substitution

hydroxide ion with bromoethane

mechanism

$CH_3CH_2Br + OH^-$ (aqueous) $\longrightarrow$ $CH_3CH_2OH + Br^-$

ethanol

hydroxide ion with 2-bromo,2-methylpropane

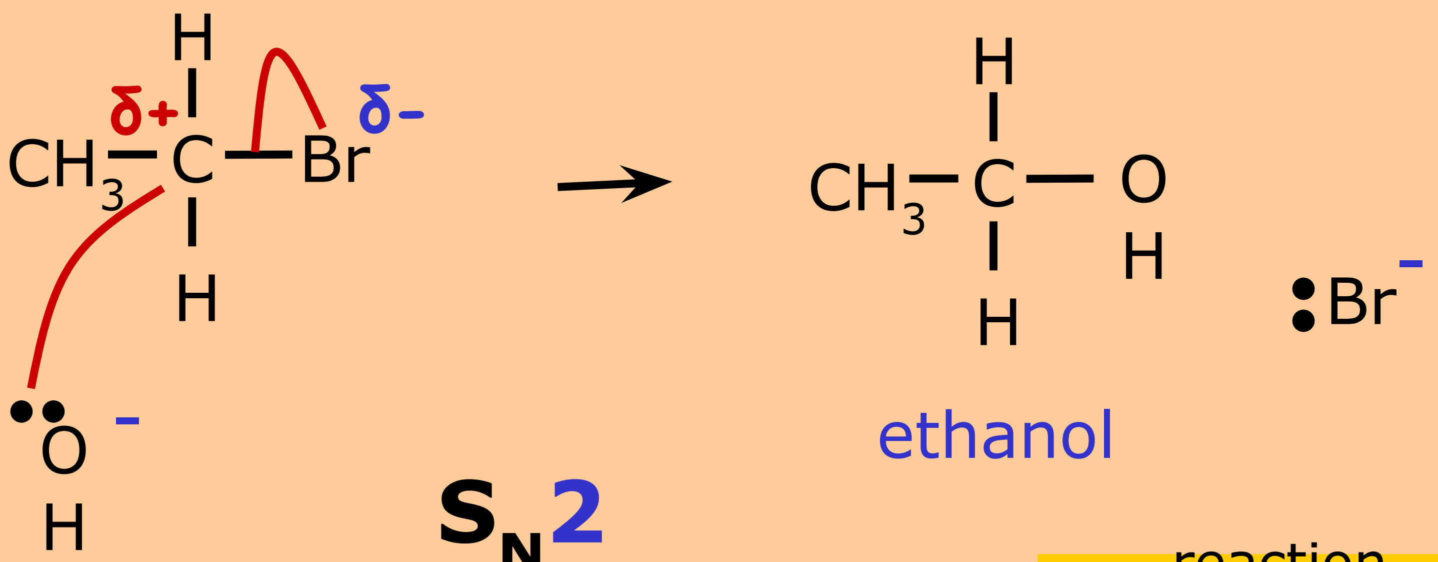
mechanism

$(CH_3)_3CBr + OH^-$ (aqueous) $\longrightarrow$ $(CH_3)_3COH + Br^-$

2-methylpropan-2-ol

Nucleophilic substitution mechanism

hydroxide ion with bromoethane (S_N2)



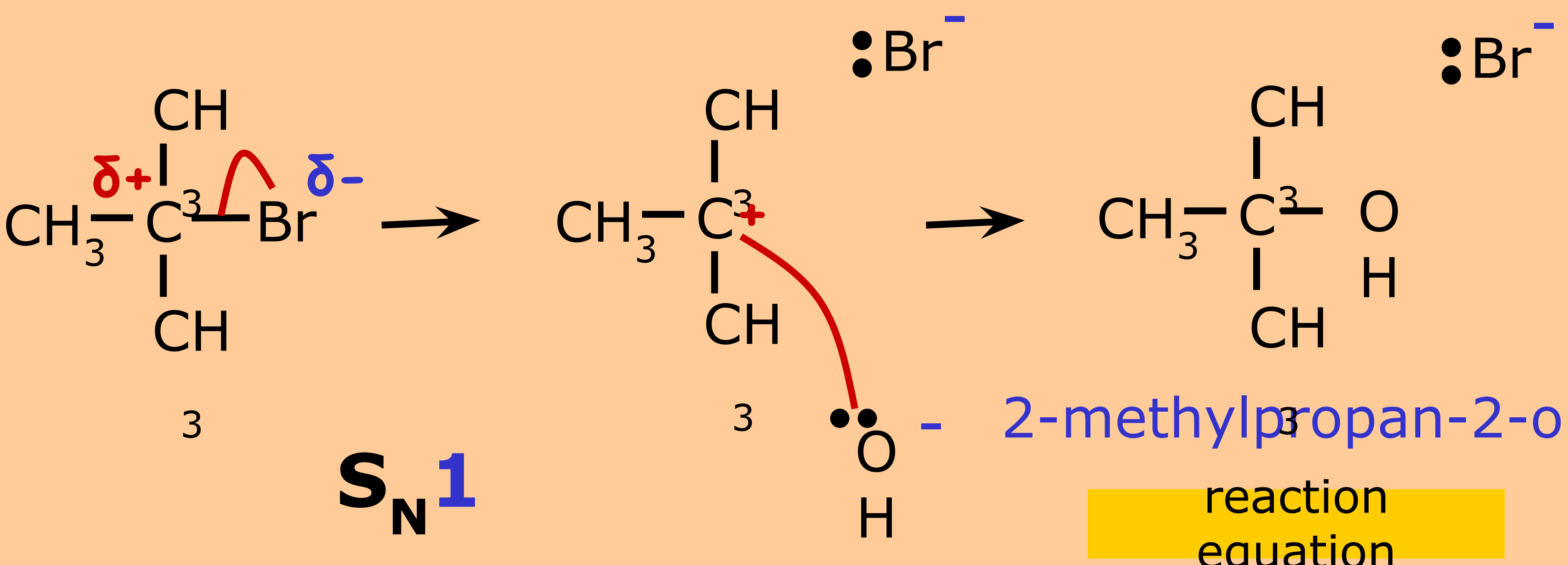
S$_N$**2**

reaction equation

S (substitution) **N** (nucleophilic) **2** (species reacting in the slowest step)

Nucleophilic substitution mechanism

OH^- ion with 2-bromo,2-methylpropane (S_N1)



S (substitution) **N** (nucleophilic) **1** (species reacting in the slowest step)

Nucleophilic substitution

cyanide ion with iodoethane

mechanism

CH_3CH_2I (ethanol) + CN^-(aq) $\longrightarrow$ $CH_3CH_2CN + I^-$

propanenitrile

cyanide ion with 2-bromo,2-methylpropane

mechanism

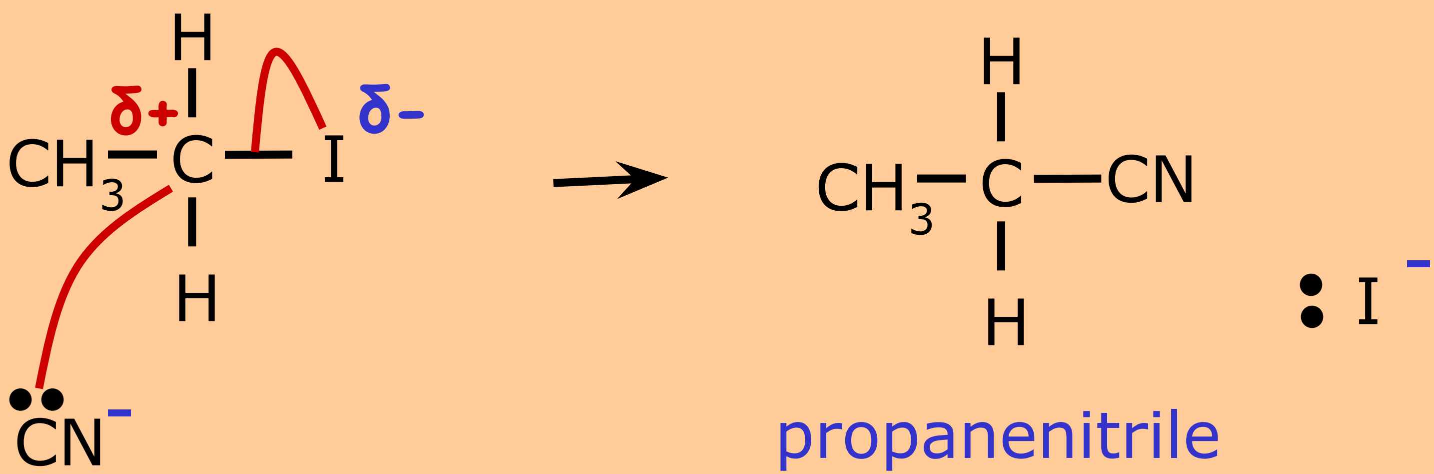
$(CH_3)_3CBr$ (ethanol) + CN^- (aqueous)

$\longrightarrow$ $(CH_3)_3CCN + Br^-$

2,2-dimethylpropanenitrile

Nucleophilic substitution mechanism

cyanide ion with iodoethane (S_N2)



propanenitrile

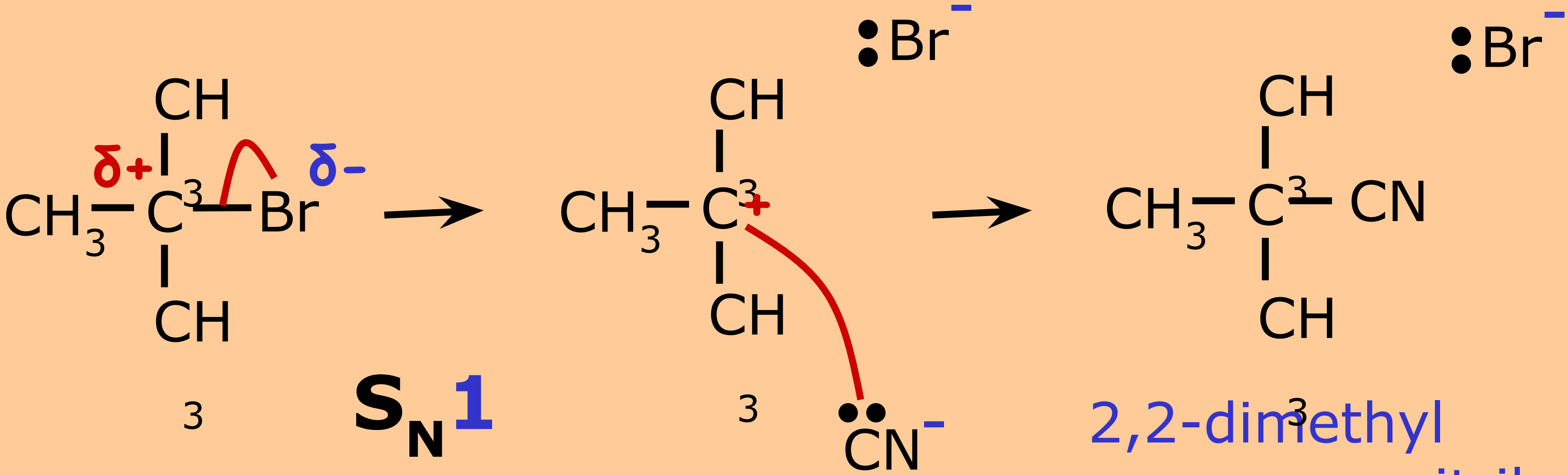
S_N2

S (substitution) **N** (nucleophilic) **2** (species reacting in the slowest step)

reaction equation

Nucleophilic substitution mechanism

CN^- ion with 2-bromo,2-methylpropane (S$_N$1)



2,2-dimethyl propanenitrile

S (substitution) **N** (nucleophilic) **1** (species reacting in the slowest step)

reaction equation

Electrophilic Substitution

Nitration of benzene

Where an H atom attached to an aromatic ring is replaced by an NO_2 group of atoms

$$C_6H_6 \quad + \quad HNO_3 \quad \longrightarrow \quad C_6H_5NO_2 \quad + \quad H_2O$$

Conditions / Reagents

concentrated HNO_3 **and** concentrated H_2SO_4

50^oC

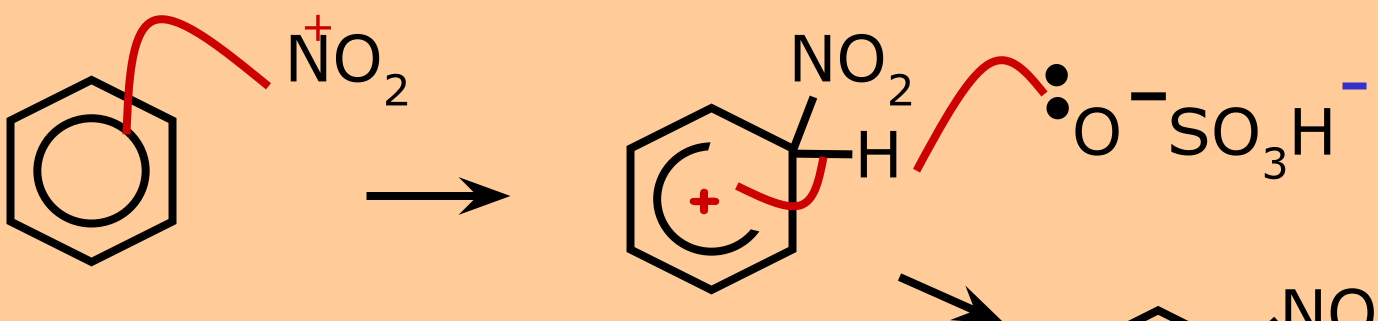
mechanism

electrophilic substitution mechanism (nitration)

1. Formation of $\overset{+}{N}O_2$ the **nitronium ion**

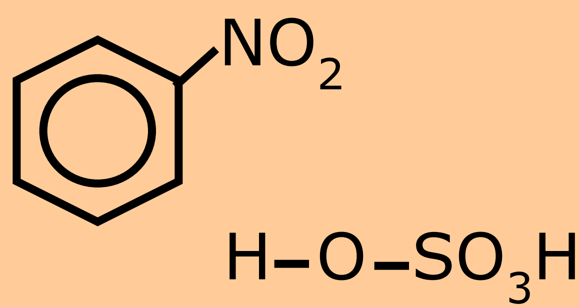
$$HNO_3 + 2H_2SO_4 \longrightarrow \overset{+}{N}O_2 + 2HSO_4^- + H_3O^+$$

2. Electrophilic attack on benzene



3. Forming the product

and re-forming the catalyst



reaction equation

Bromination of benzene

Where an H atom attached to an aromatic ring is replaced by a Br atom

electrophilic substitution

$$C_6H_6 \quad + \quad Br_2 \longrightarrow C_6H_5Br \quad + \quad HBr$$

R = alkyl group

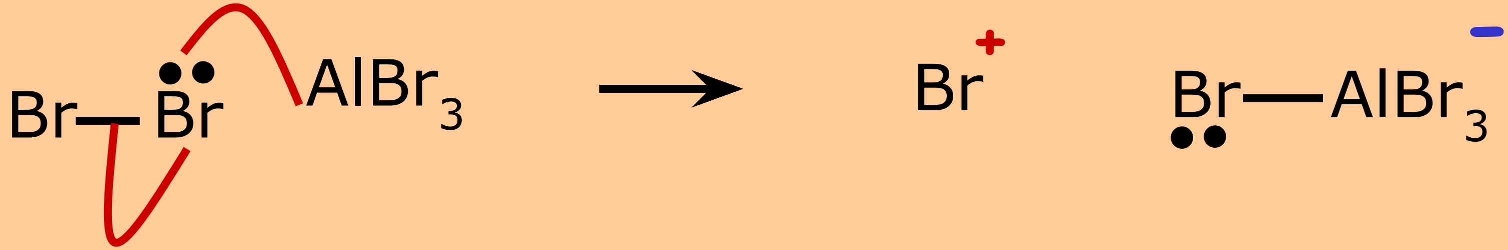
Conditions / Reagents

Br_2 **and** anhydrous $AlBr_3$

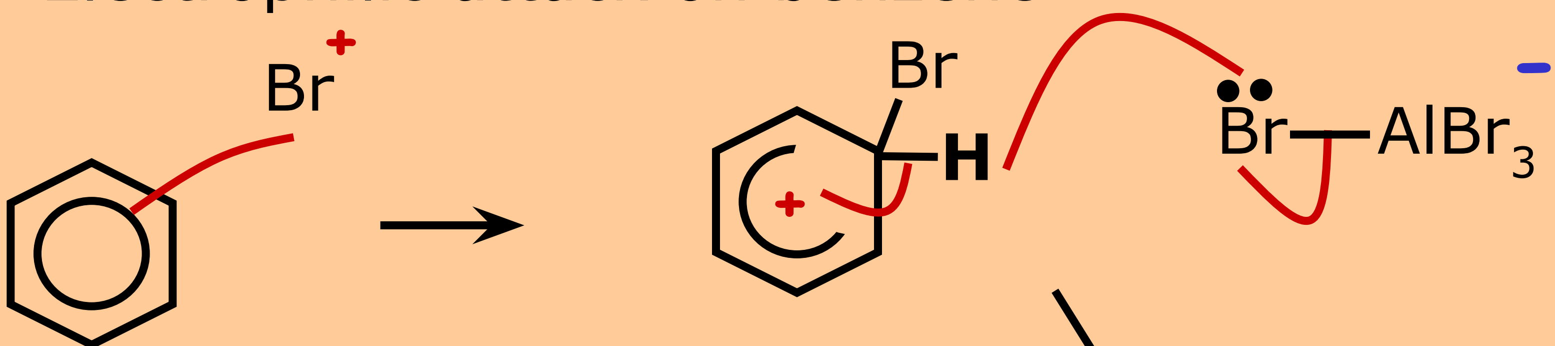
25^oC

Electrophilic substitution mechanism

1. Formation of the electrophile

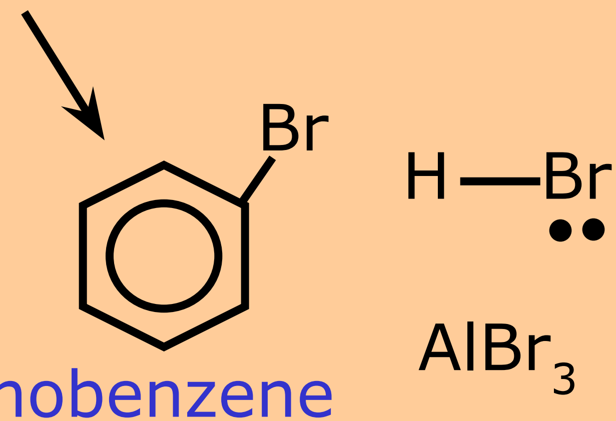


2. Electrophilic attack on benzene



3. Forming the products

and re-forming the catalyst



Alkylation of benzene

Where an H atom attached to an aromatic ring is replaced by a C atom

electrophilic substitution

$$C_6H_6 \quad + \quad RCl \longrightarrow C_6H_5R \quad + \quad HCl$$

R = alkyl group

Conditions / Reagents

RCl (haloakane) **and** anhydrous $AlCl_3$

0 - 25°C to prevent further substitution

Alkylation example

With chloroethane **overall reaction equation**

$$C_6H_6 + CH_3CH_2Cl \longrightarrow C_6H_5CH_2CH_3 + HCl$$

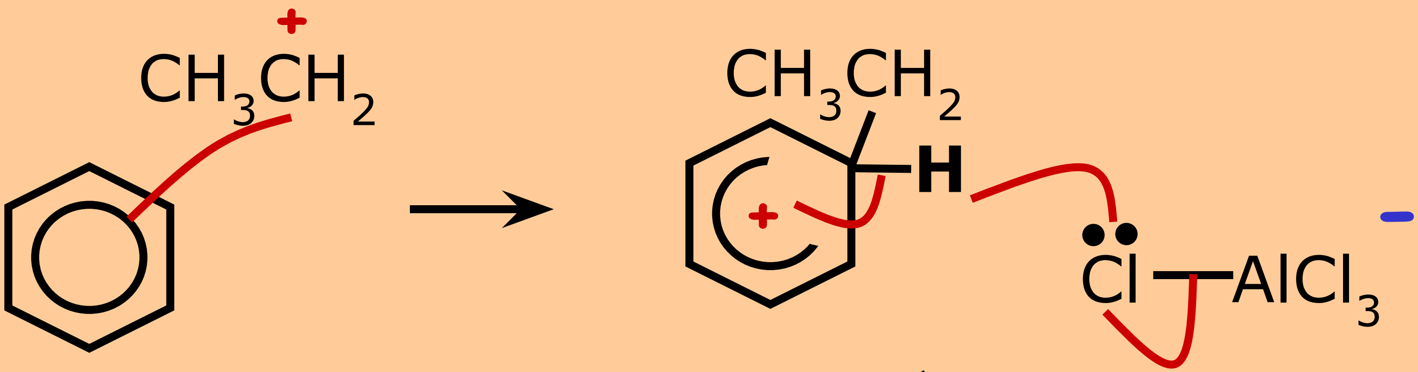
Three steps in electrophilic substitution mechanism

1. Formation of the electrophile (a **carbocation**)

$$CH_3CH_2{-}Cl \quad AlCl_3 \longrightarrow CH_3\overset{+}{C}H_2 \quad Cl{-}AlCl_3^{\,-}$$

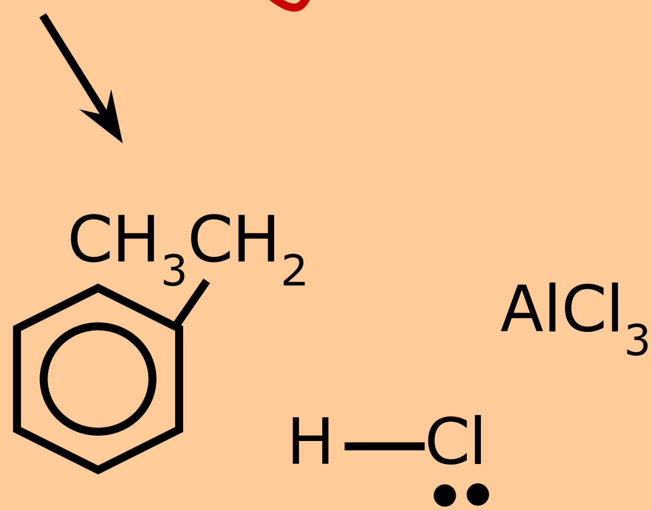
Alkylation electrophilic substitution mechanism 2

2. Electrophilic attack on benzene



3. Forming the product

and re-forming the catalyst



ethylbenzene

Acylation of benzene

An H atom attached to an aromatic ring
is replaced by a C atom where C is part of C=O

electrophilic substitution

$$C_6H_6 + RCOCl \longrightarrow C_6H_5COR + HCl$$

Conditions / Reagents

RCOCl (acyl chloride) **and** anhydrous $AlCl_3$

50 °C

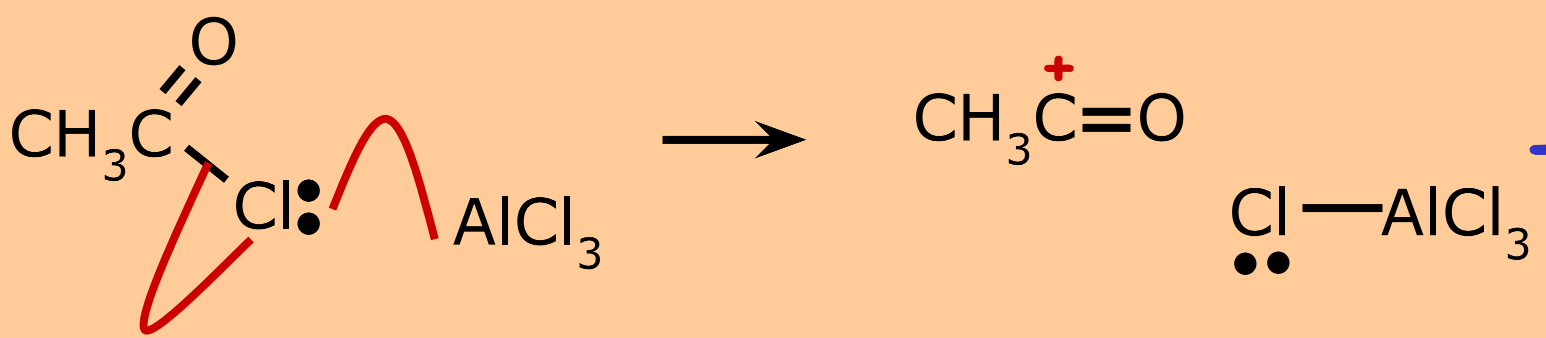
Acylation example

With ethanoyl chloride **overall reaction equation**

$$C_6H_6 + CH_3COCl \longrightarrow C_6H_5COCH_3 + HCl$$

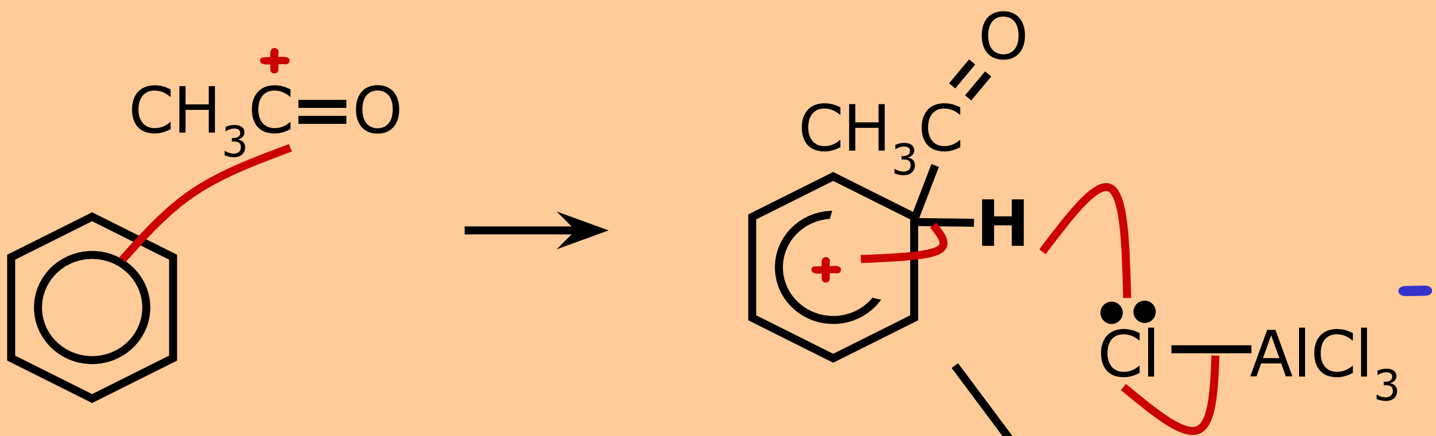
Three steps in electrophilic substitution mechanism

1. Formation of the electrophile (an **acylium** ion)



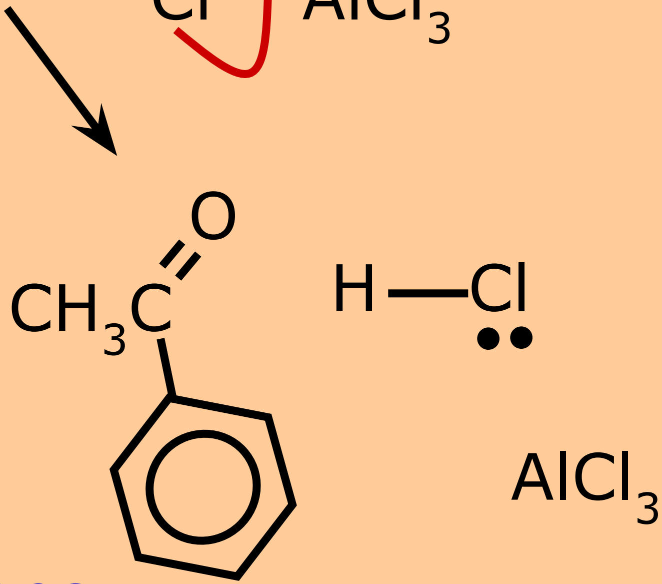
Acylation electrophilic substitution mechanism 2

2. Electrophilic attack on benzene



3. Forming the products

and re-forming the catalyst



phenylethanone

Nucleophilic Addition

addition of hydrogen cyanide to carbonyls to form hydroxynitriles

$$RCOR + HCN \longrightarrow RC(OH)(CN)R$$

$$RCHO + HCN \longrightarrow RCH(OH)CN$$

Conditions / Reagents

NaCN (aq) and H_2SO_4(aq) supplies H^+
supplies the CN^- nucleophile

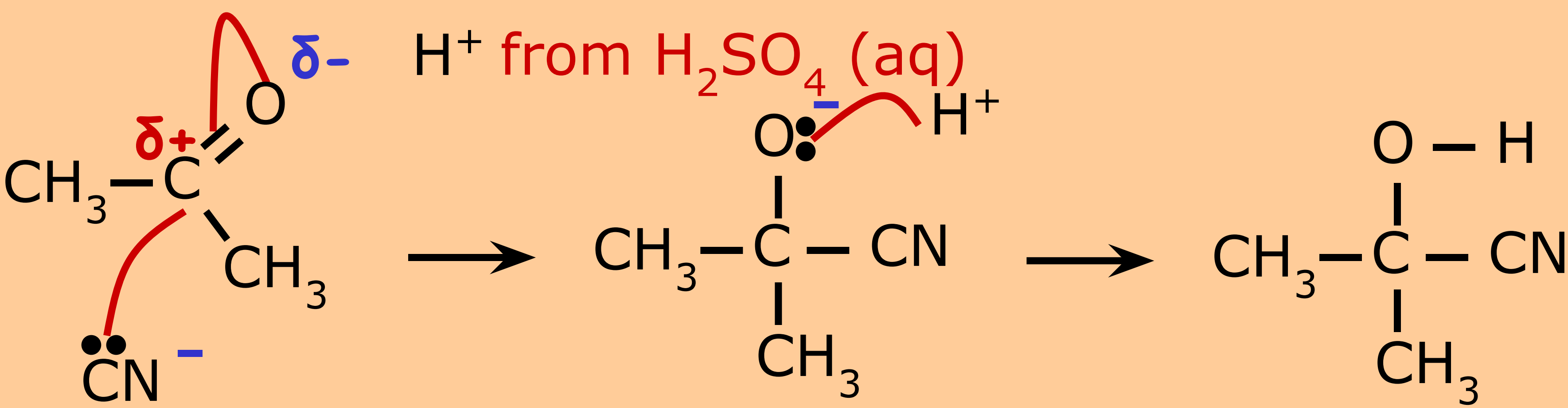
Room temperature and pressure

Nucleophilic Addition Mechanism

hydrogen cyanide with propanone

$$CH_3COCH_3 \; + \; HCN \longrightarrow CH_3C(OH)(CN)CH_3$$

NaCN (aq) is a source of **cyanide ions** $:C\equiv N^{-}$



2-hydroxy-2-methylpropanenitrile

Advice

To get back to the mechanism links page from anywhere in the presentation, click the button at the top right corner of the screen.

This version provides the organic mechanisms specified (2002/3) by the Edexcel exam board. Each stage of a reaction equation, its conditions and mechanism are revealed in turn on a mouse click or keyboard stroke. Note that there is another version available where each reaction and mechanism play automatically after an initiating click or key stroke.

The number of ways of navigating through this presentation may depend on the version of PowerPoint being used and how it is configured.

Some possible ways of advancing:

left mouse click or return key or right arrow key or up arrow key.

Some possible ways of reversing:

backspace key or left arrow key or down arrow key.

References

Steve Lewis for the Royal Society of Chemistry