

9 Compound **X** is made from benzene by the route shown in Fig. 9.1.

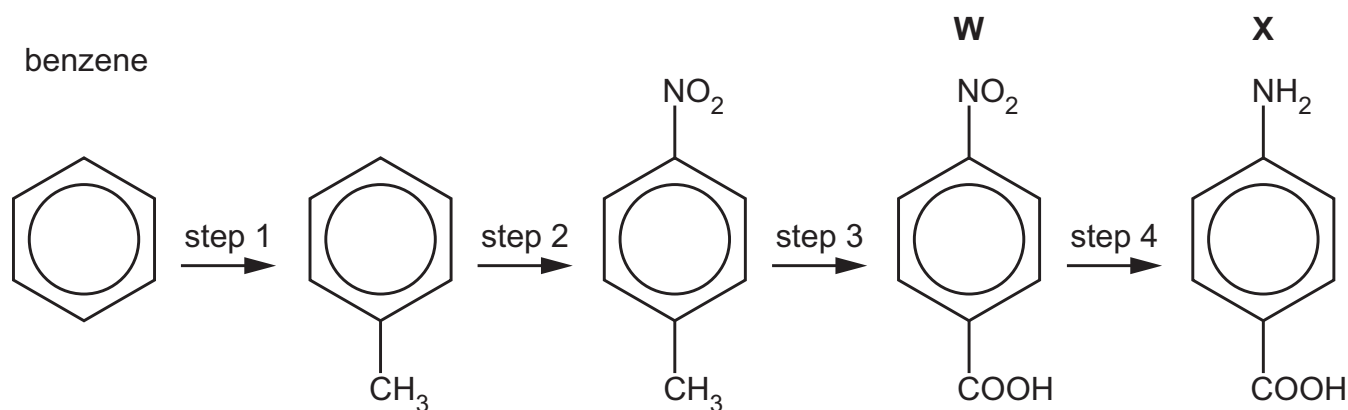


Fig. 9.1

(a) Describe the bonding in benzene, C_6H_6 .

Your answer should include:

- the hybridisation of the six carbon atoms
- the types of bond between the carbon atoms
- the orbitals that overlap to produce the bonds between the carbon atoms
- the type of bond between the carbon atoms and the hydrogen atoms
- the orbitals that overlap to produce the bonds between the carbon atoms and the hydrogen atoms.

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..... [3]

(b) Describe the reagents and conditions required for step 1 in Fig. 9.1.

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..... [1]

(c) In step 1 of Fig. 9.1 benzene reacts with $^+\text{CH}_3$.

Complete Fig. 9.2 to show the mechanism for this reaction, including:

- the movement of electron pairs using curly arrows
- the structure of the intermediate involved.

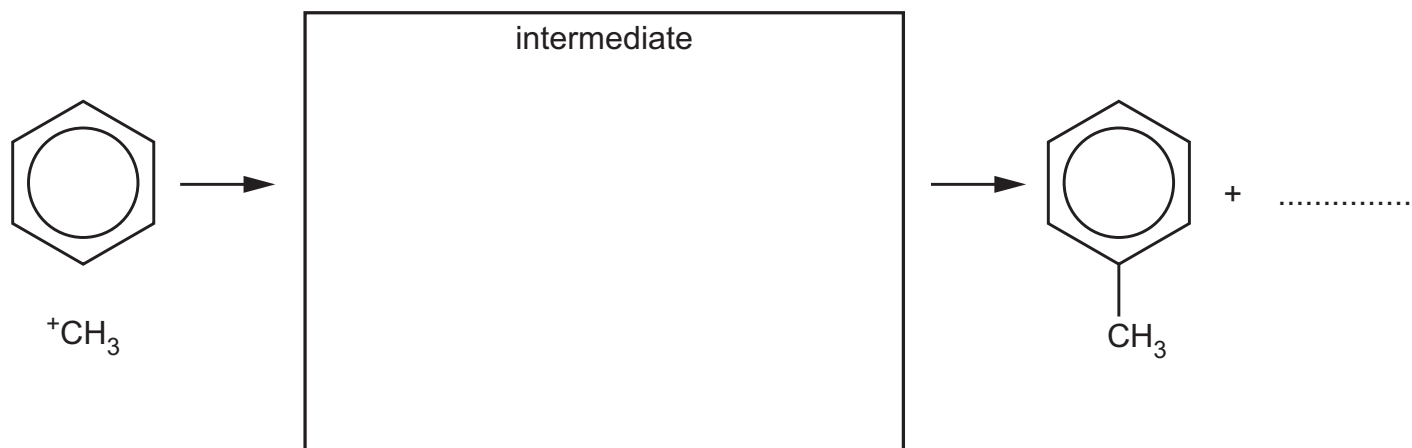


Fig. 9.2

[3]

(d) Describe the reagents and conditions required for step 2 of Fig. 9.1.

.....
..... [2]

(e) Identify the reagents required for step 3 of Fig. 9.1. Compound **W** is the product of this step.

..... [1]

(f) Name compound **W**.

..... [1]

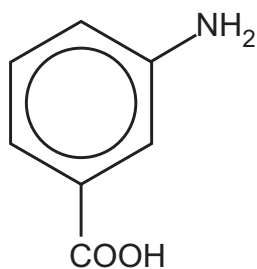
(g) The reagents commonly used for step 4 will **not** reduce the $-\text{COOH}$ group.

Identify the reagents and conditions required for step 4 of Fig. 9.1.

..... [1]

(h) Benzene can also be used as a starting material to make compound **Y**.

compound **Y**



Describe how the route described in Fig. 9.1 (repeated below) can be changed to give compound **Y** instead of compound **X**.

Explain your answer.

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..... [2]

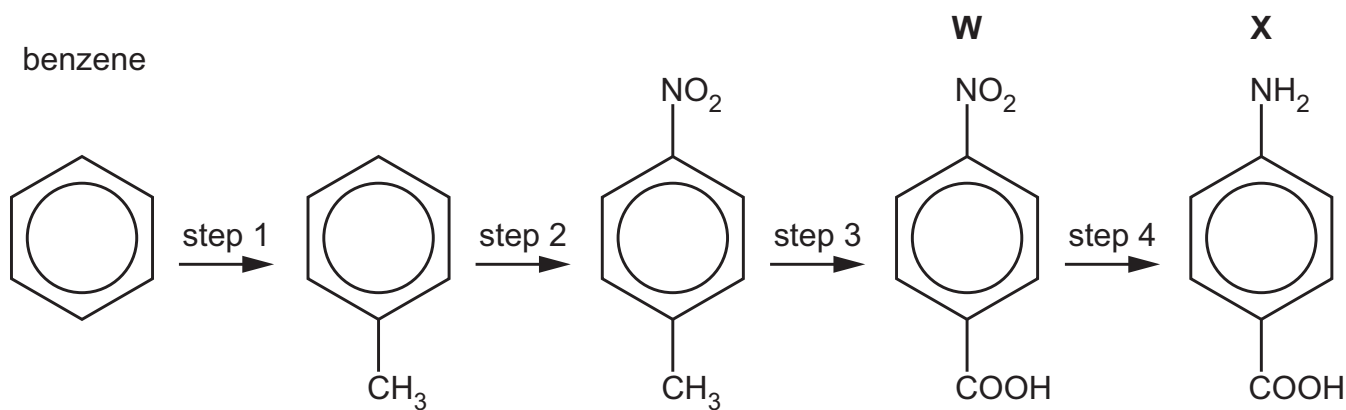


Fig. 9.1

[Total: 14]

Important values, constants and standards

molar gas constant	$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
Faraday constant	$F = 9.65 \times 10^4 \text{ C mol}^{-1}$
Avogadro constant	$L = 6.02 \times 10^{23} \text{ mol}^{-1}$
electronic charge	$e = -1.60 \times 10^{-19} \text{ C}$
molar volume of gas	$V_m = 22.4 \text{ dm}^3 \text{ mol}^{-1}$ at s.t.p. (101 kPa and 273 K) $V_m = 24.0 \text{ dm}^3 \text{ mol}^{-1}$ at room conditions
ionic product of water	$K_w = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$ (at 298 K (25 °C))
specific heat capacity of water	$c = 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ (4.18 J g ⁻¹ K ⁻¹)

8 (a) In the electrophilic substitution of arenes, different substituents can direct to different ring positions.

(i) Describe the directing effect of the -NO_2 group. Explain your answer.

.....
..... [1]

(ii) The nitration of arenes uses a mixture of concentrated HNO_3 and concentrated H_2SO_4 to generate the NO_2^+ electrophile.

Write an equation for the formation of the NO_2^+ electrophile.

..... [1]

(b) Carbon-carbon bond formation is an important reaction in organic synthesis.

Fig. 8.1 shows the synthesis of compound **Q** from benzene in two reaction steps.

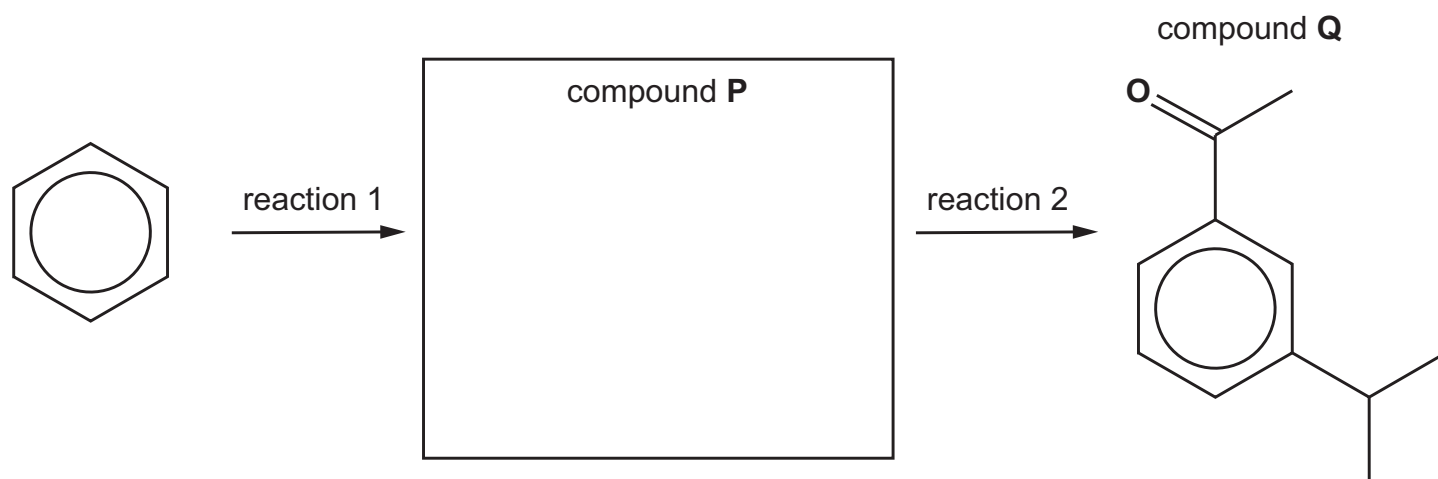


Fig. 8.1

(i) Draw the structure of compound **P** in the box in Fig. 8.1.

[1]

(ii) Suggest reagents and conditions for reactions 1 and 2 in Fig. 8.1.

reaction 1

reaction 2

[2]

(c) Separate samples of $\text{C}_6\text{H}_5\text{Br}$ and $\text{C}_6\text{H}_5\text{CH}_2\text{Br}$ are added to warm $\text{AgNO}_3(\text{aq})$.

State the expected observations, if any. Explain your answer.

$\text{C}_6\text{H}_5\text{Br}$ with $\text{AgNO}_3(\text{aq})$

$\text{C}_6\text{H}_5\text{CH}_2\text{Br}$ with $\text{AgNO}_3(\text{aq})$

explanation

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.....

.....

[3]

(d) Acyl bromides, RCOBr , react readily with H_2O .

The mechanism of this reaction is similar to that of the reaction of H_2O with acyl chlorides, RCOCl .

(i) Name the mechanism of this reaction.

..... [1]

(ii) Complete the mechanism in Fig. 8.2 for the reaction of RCOBr with H_2O .

Include all relevant lone pairs of electrons, curly arrows, charges and dipoles.

Draw the structure of the intermediate.

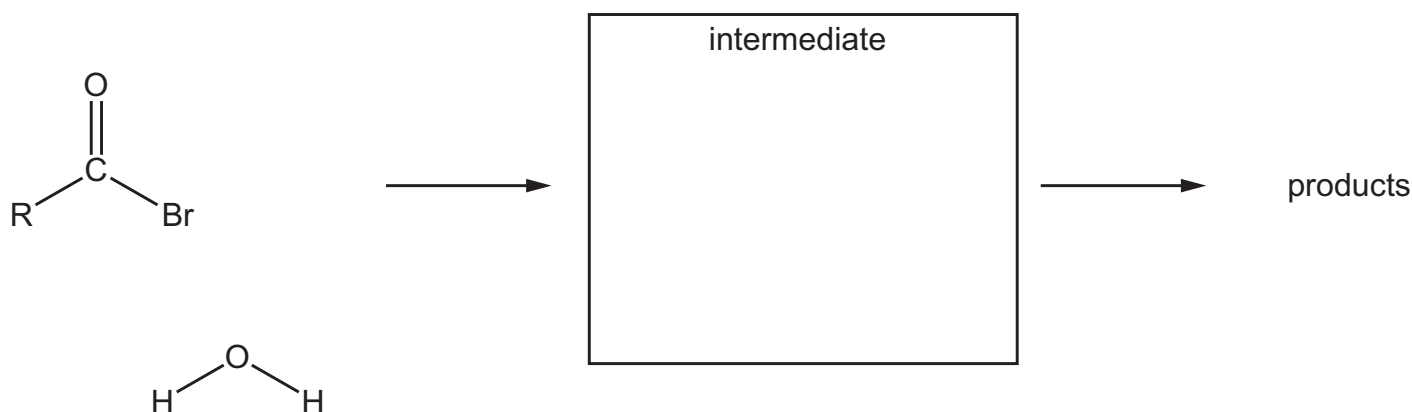


Fig. 8.2

[4]

[Total: 13]

5 (a) Describe and explain the shape of benzene.

In your answer, include:

- the shape and bond angle in the ring
- the hybridisation of the carbon atoms
- how orbital overlap forms σ and π bonds between the carbon atoms in the ring.

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..... [4]

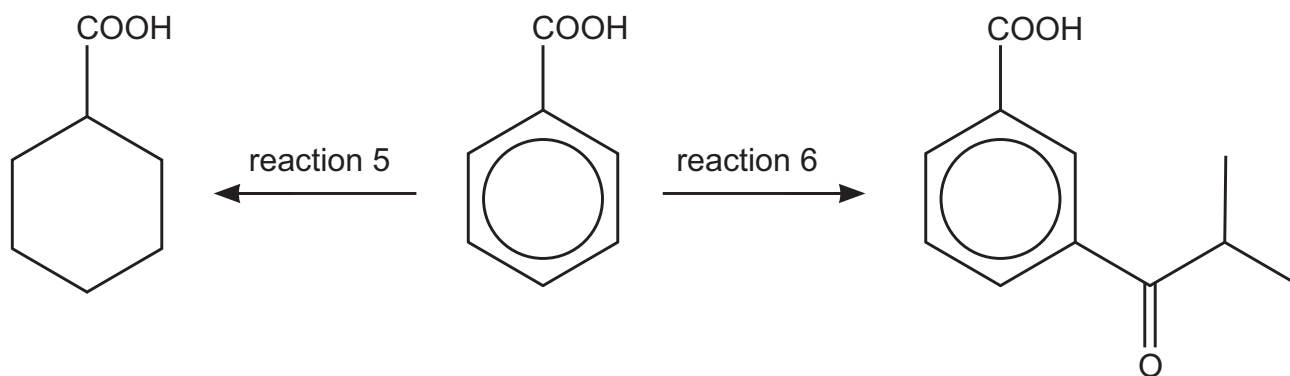
(b) Fig. 5.1 shows two reactions of benzoic acid.

Fig. 5.1

(i) Suggest reagents and conditions for reaction 5 and for reaction 6 in Fig. 5.1.

reaction 5

reaction 6

[2]

(ii) State the type of reaction for reaction 5 in Fig. 5.1.

..... [1]

(c) In the electrophilic substitution of arenes, different substituents can direct to different ring positions.

(i) Describe the directing effect of the $-\text{CH}_2\text{CH}_3$ group.

Explain your answer.

.....
..... [1]

(ii) The alkylation of arenes uses a mixture of $\text{CH}_3\text{CH}_2\text{Br}$ and FeBr_3 to generate the CH_3CH_2^+ electrophile.

Write an equation for the formation of the CH_3CH_2^+ electrophile.

..... [1]

(iii) Complete the mechanism in Fig. 5.2.

Include all relevant curly arrows and charges. Draw the structure of the organic intermediate.

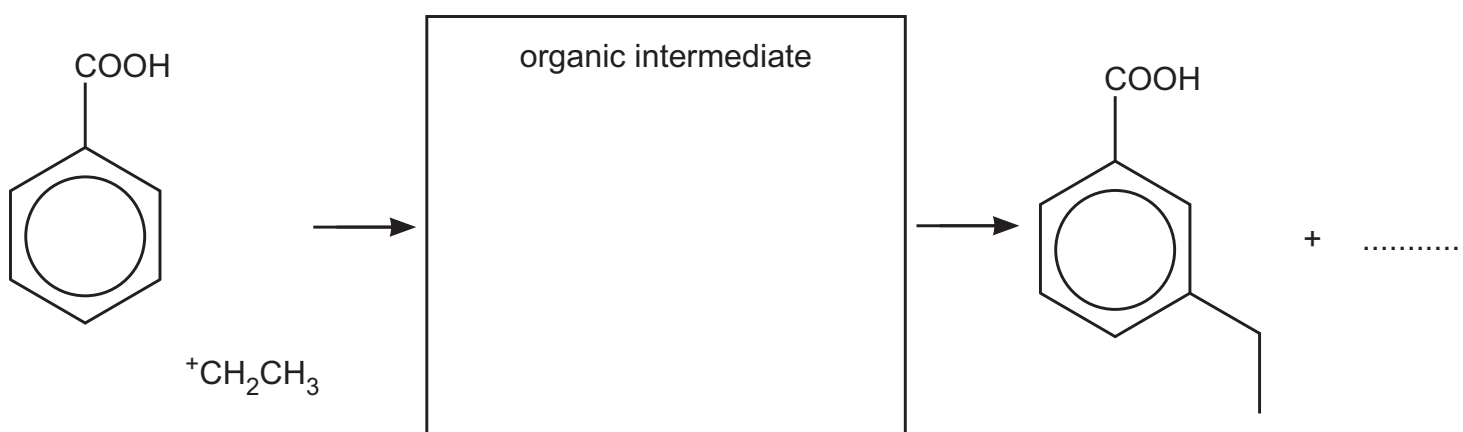


Fig. 5.2

[3]

(iv) Write an equation to show how FeBr_3 is regenerated after the reaction in Fig. 5.2.

..... [1]

[Total: 13]