

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

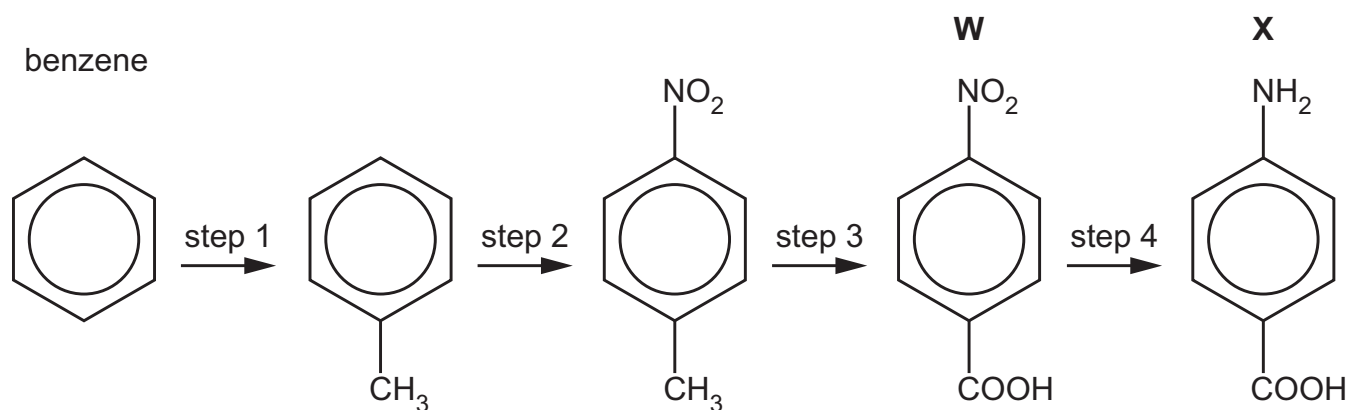


Fig. 9.1

(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.

.....

..... [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.

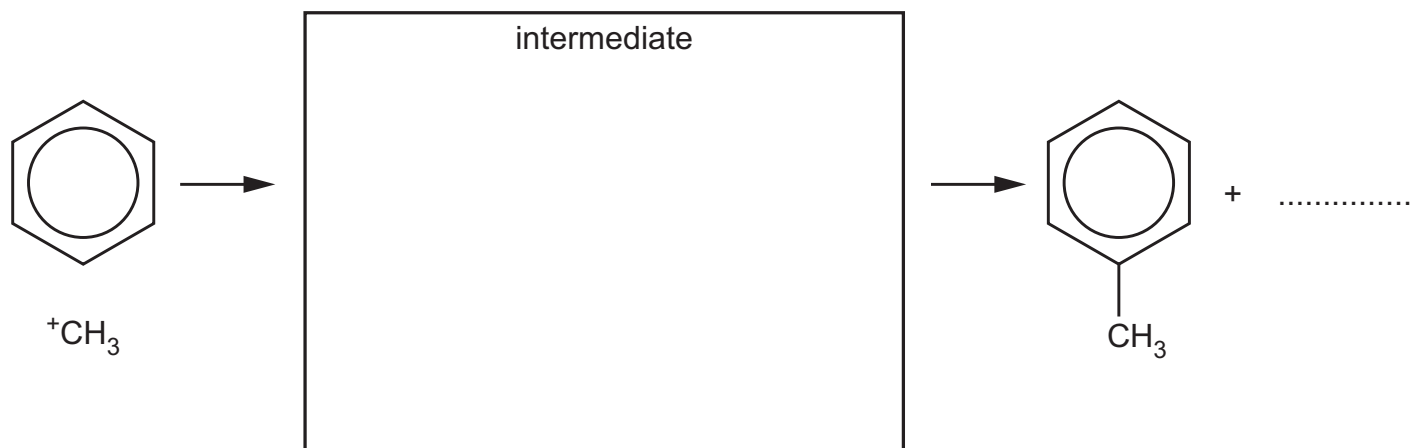


Fig. 9.2

[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]

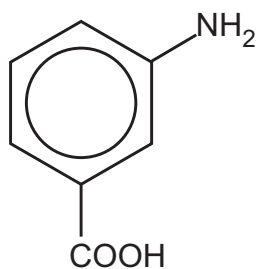
(g) The reagents commonly used for step 4 will **not** reduce the $-\text{COOH}$ group.

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]

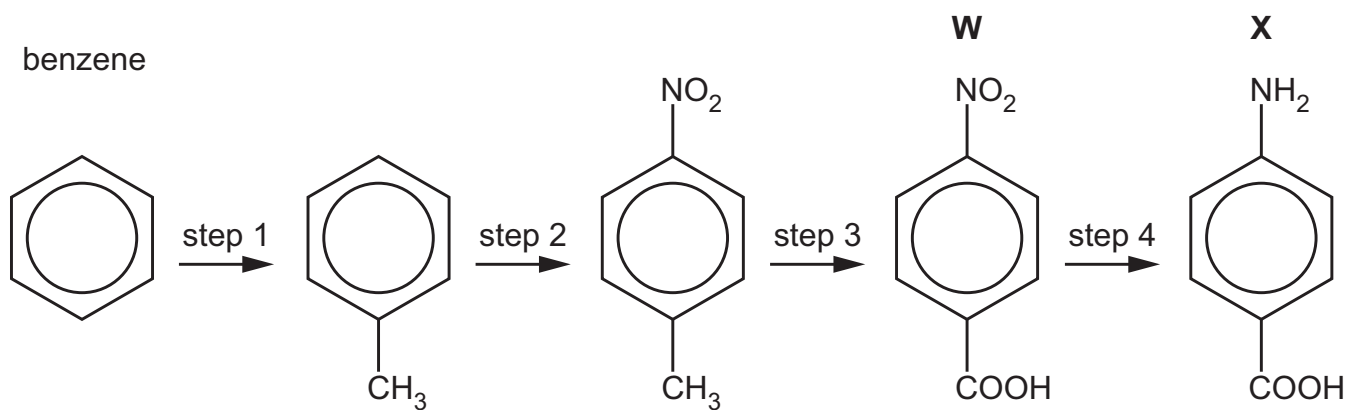


Fig. 9.1

[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)

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]

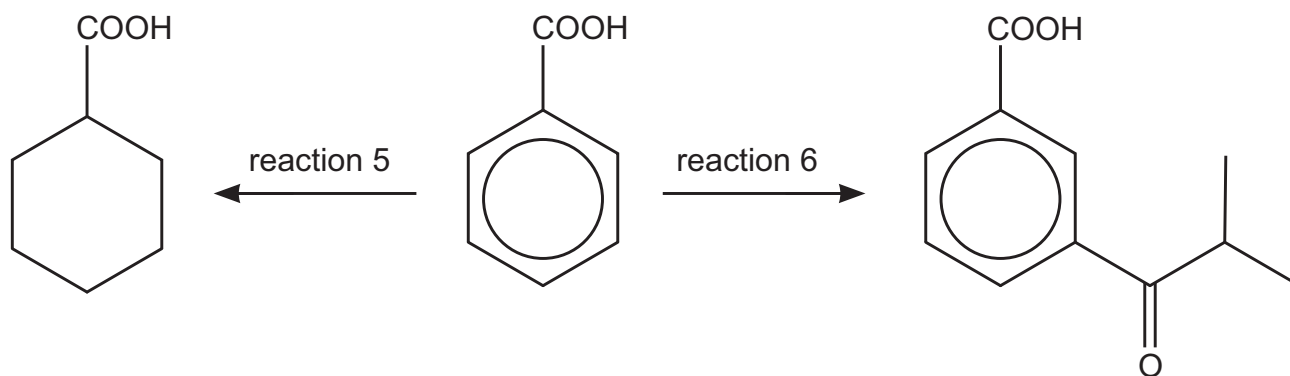
(b) Fig. 5.1 shows two reactions of benzoic acid.

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.

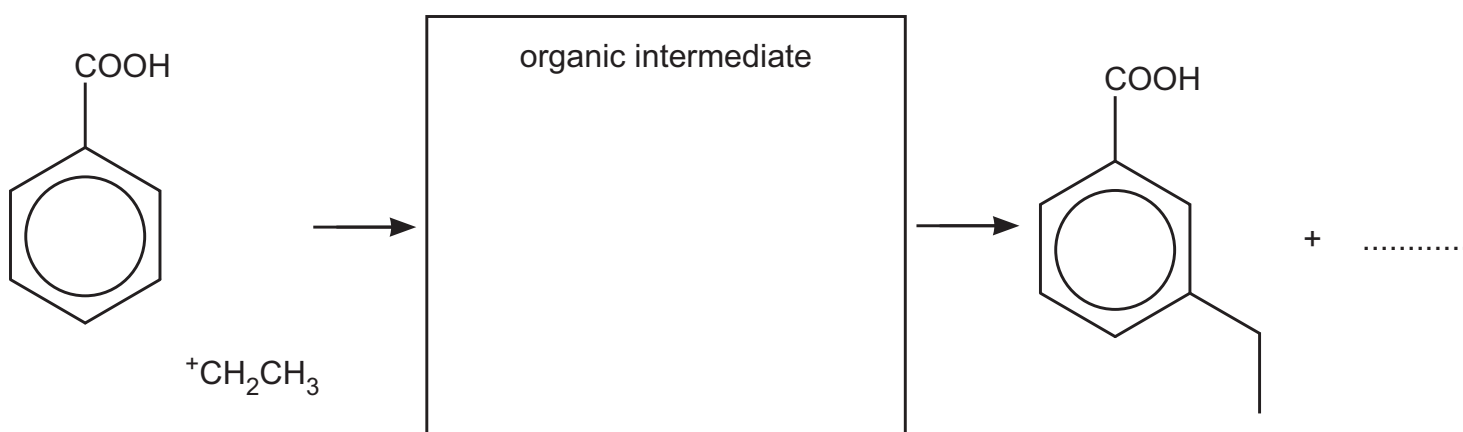


Fig. 5.2

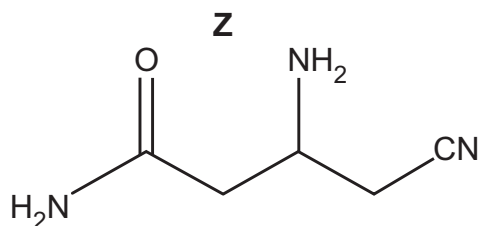
[3]

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

..... [1]

[Total: 13]

6 (a) Compound **Z** is used in organic synthesis.



Complete Table 6.1 to show the number of sp , sp^2 and sp^3 hybridised carbon atoms present in one molecule of **Z**.

Table 6.1

type of hybridisation	sp	sp^2	sp^3
number of carbon atoms			

[1]

(b) **Z** can undergo different reactions, as shown in Fig. 6.1.

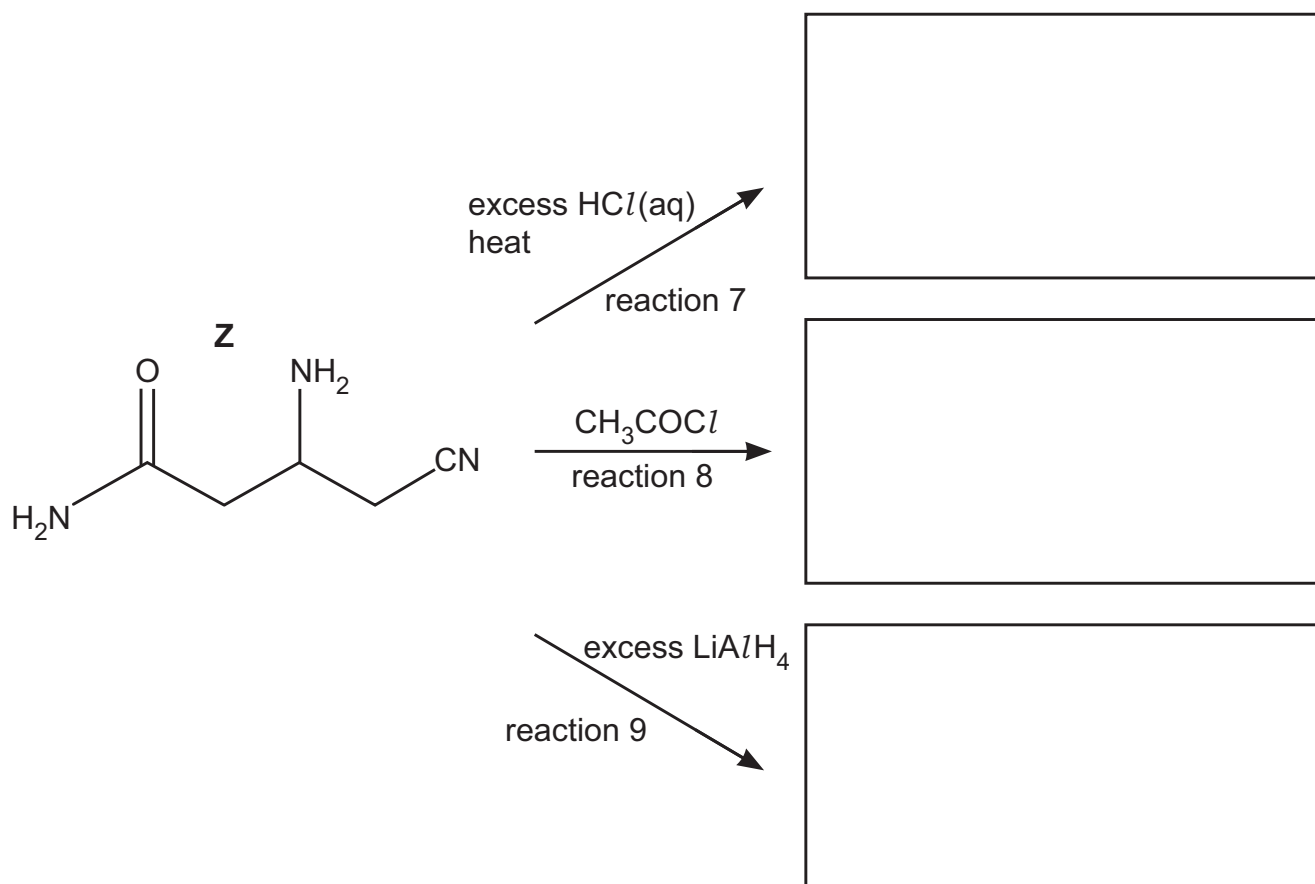


Fig. 6.1

(i) Name the **two** types of reaction occurring in reaction 7 in Fig. 6.1.

..... and [1]

(ii) Draw the structures of the organic products of reactions 7, 8 and 9 in Fig. 6.1.

[4]

(c) Compound **Z** is dissolved in D₂O and analysed by carbon-13 NMR and proton (¹H) NMR spectroscopy.

(i) Predict the number of peaks in the carbon-13 NMR spectrum of **Z**.

..... [1]

(ii) The proton (¹H) NMR spectrum of **Z** in D₂O gives three peaks for the proton environments, labelled **a**, **b** and **c**, as shown on Fig. 6.2.

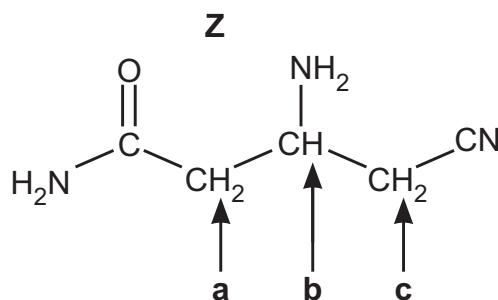


Fig. 6.2

Complete Table 6.2 for the proton (¹H) NMR spectrum of **Z** in D₂O.

Table 6.2

proton environment	a	b	c
name of splitting pattern			
chemical shift range, δ /ppm			

[2]

Table 6.3

environment of proton	example	chemical shift range, δ /ppm
alkane	$-\text{CH}_3$, $-\text{CH}_2-$, $>\text{CH}-$	0.9–1.7
alkyl next to C=O	$\text{CH}_3-\text{C}=\text{O}$, $-\text{CH}_2-\text{C}=\text{O}$, $>\text{CH}-\text{C}=\text{O}$	2.2–3.0
alkyl next to nitrile	$-\text{CH}_2-\text{CN}$	2.0–3.0
alkyl next to electronegative atom	CH_3-O , $-\text{CH}_2-\text{O}$, $-\text{CH}_2-\text{N}$	3.2–4.0
attached to alkene	$=\text{CHR}$	4.5–6.0
alkyl amine	$\text{R}-\text{NH}-$	1.0–5.0
amide	RCONHR	5.0–12.0

[Total: 9]