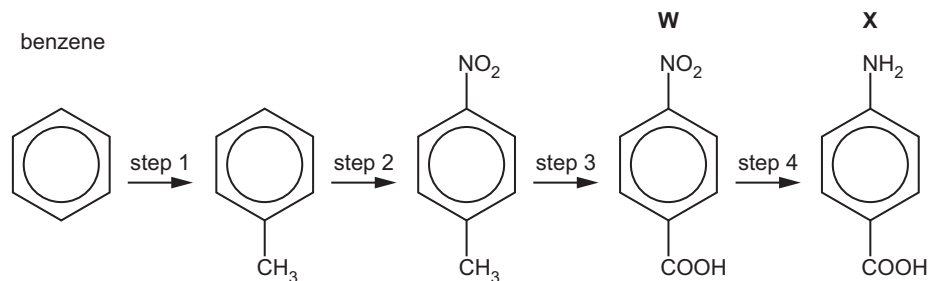


9 Compound **X** is made from benzene by the route shown in Fig. 9.1.



(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.

.....
.....
.....
.....
.....
..... [3]

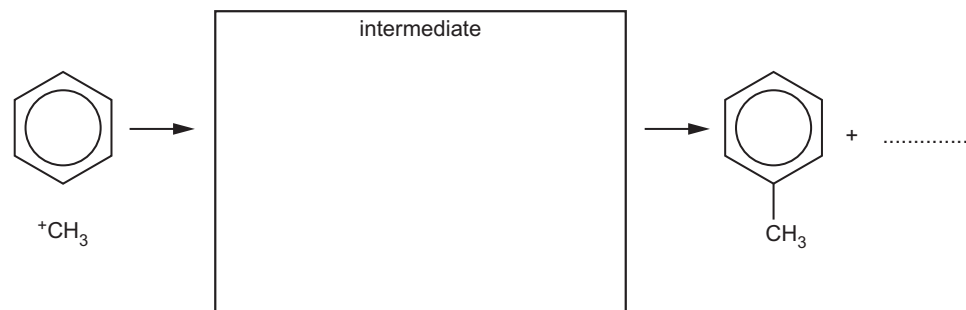
(b) Describe the reagents and conditions required for step 1 in Fig. 9.1.

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

(c) In step 1 of Fig. 9.1 benzene reacts with $^+CH_3$.

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.



[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]

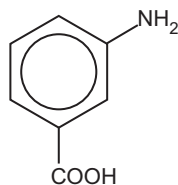
(g) The reagents commonly used for step 4 will **not** reduce the $-COOH$ group.

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**

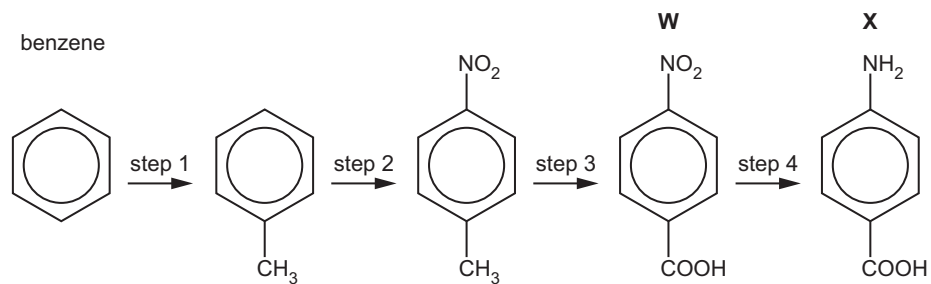


Describe how the route described in Fig. 9.1 (repeated below) can be changed to give compound **Y** instead of compound **X**.

Explain your answer.

.....

 [2]



[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	$c = 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ ($4.18 \text{ J g}^{-1} \text{ K}^{-1}$)

The Periodic Table of Elements

Group																				
1	2	Key														17	18			
3	4	atomic number atomic symbol relative atomic mass												5	6	7	8	9	2	
Li lithium 6.9	Be beryllium 9.0													H hydrogen 1.0	B boron 10.8	C carbon 12.0	N nitrogen 14.0	O oxygen 16.0	F fluorine 19.0	He helium 4.0
11	12													13	14	15	16	17	18	
Na sodium 23.0	Mg magnesium 24.3													Al aluminum 27.0	Si silicon 28.1	P phosphorus 31.0	S sulfur 32.1	Cl chlorine 35.5	Ar argon 39.9	
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36			
K potassium 39.1	Ca calcium 40.1	Sc scandium 45.0	Ti titanium 47.9	V vanadium 50.9	Cr chromium 52.0	Mn manganese 54.9	Fe iron 55.8	Co cobalt 58.9	Ni nickel 58.7	Cu copper 63.5	Zn zinc 65.4	Ga gallium 69.7	Ge germanium 72.6	As arsenic 74.9	Se selenium 79.0	Br bromine 79.9	Kr krypton 83.8			
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54			
Rb rubidium 85.5	Sr strontium 87.6	Y yttrium 88.9	Zr zirconium 91.2	Nb niobium 92.9	Mo molybdenum 95.9	Tc technetium —	Ru ruthenium 101.1	Rh rhodium 106.4	Pd palladium 106.4	Ag silver 107.9	Cd cadmium 112.4	In indium 114.8	Sn tin 118.7	Sb antimony 121.8	Te tellurium 127.6	I iodine 126.9	Xe xenon 131.3			
55	56	lanthanoids					72	73	74	75	76	77	78	79	80	81	82			
Cs caesium 132.9	Ba barium 137.3						Hf hafnium 178.5	Ta tantalum 180.9	W tungsten 183.8	Re rhenium 186.2	Os osmium 190.2	Pt platinum 195.1	Au gold 197.0	Hg mercury 200.6	Tl thallium 204.4	Pb lead 207.2	Bi bismuth 209.0			
87	88	actinoids					104	105	106	107	108	109	110	111	112	113	114	115		
Fr francium —	Ra radium —						Rf rutherfordium —	Db dubnium —	Sg seaborgium —	Bh bohrium —	Hs hassium —	Ds darmstadtium —	Rg roentgenium —	Cn copernicium —	Nh nihonium —	Fl flerovium —	Lv livermorium —	Ts tennessine —	Og oganeson —	

lanthanoids

actinoids

57	La	lanthanum	138.9	58	Ce	cerium	140.1	59	Pr	praseodymium	140.9	60	Nd	neodymium	144.2	61	Pm	promethium		62	Sm	samarium	150.4	63	Eu	eucadium	152.0	64	Gd	gadolinium	157.3	65	Tb	terbium	158.9	66	Dy	dysprosium	162.5	67	Ho	holmium	164.9	68	Er	erbium	167.3	69	Tm	thulium	168.9	70	Yb	ytterbium	173.0	71	Lu	lutetium	175.0				
88	Ac	actinium		89	Pa	protactinium	231.0	90	Th	thorium	232.0	91	U	uranium	238.0	92	Np	neptunium		93	Pu	plutonium		94	Am	americium		95	Cm	curium		96	Bk	berkelium		97	Cf	californium		98	Es	einsteinium		99	Fm	fermium		100	Md	meitnerium		101	Md	moscovium		102	No	nobelium		103	Lr	lawrencium	

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.

[4]

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

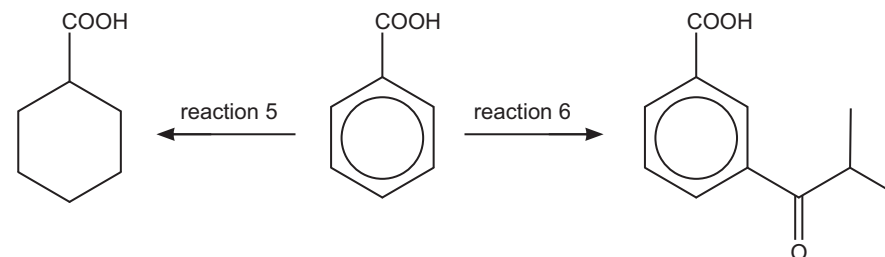


Fig. 5.1

(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.

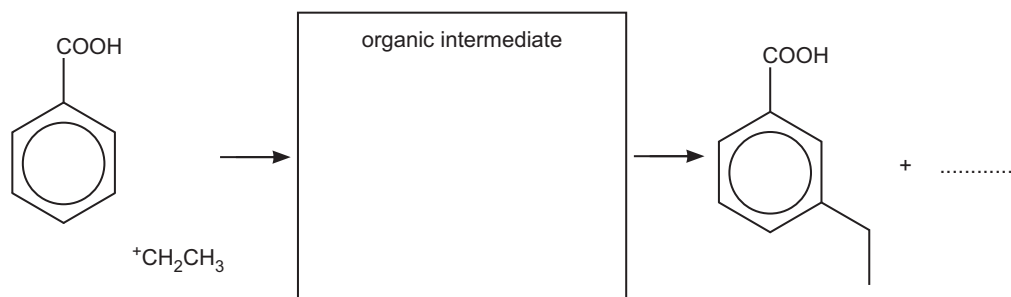


Fig. 5.2

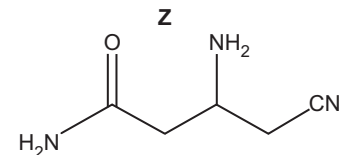
[3]

(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.

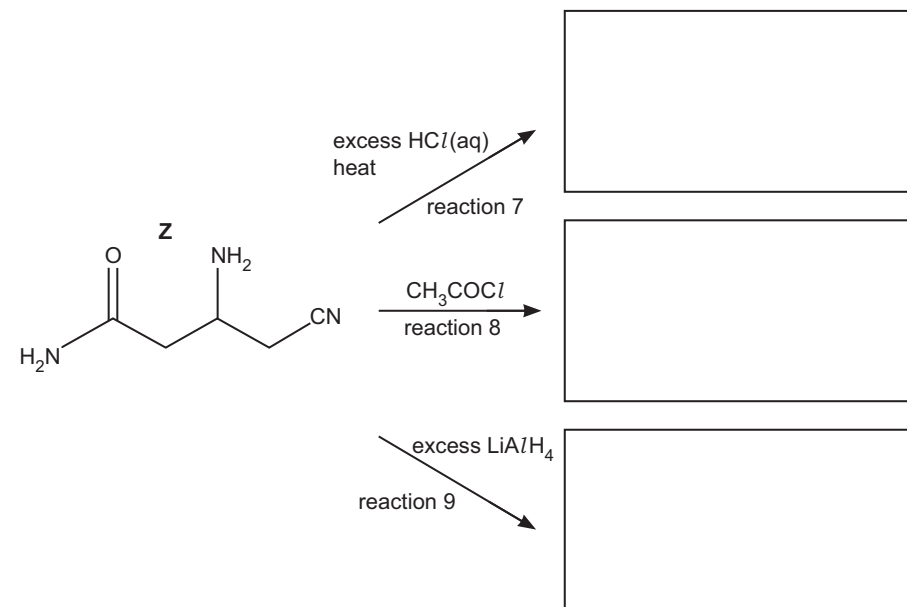


Fig. 6.1

(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.

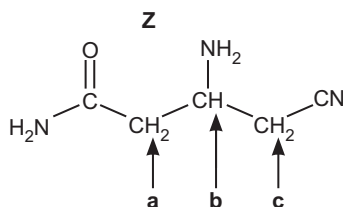


Fig. 6.2

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]