Past-paper walk-through

Shapes of aromatic organic molecules; σ and π bonds ▪ 29.3

eXercise

Questions in this set

- 9701/42 N25 Q9 ▪ 14 marks
- 9701/44 N25 Q5 ▪ 13 marks
- 9701/44 N25 Q6 ▪ 9 marks

Reading the mark scheme

- **B1** a mark that stands on its own – the point is either made or not.
- **M1** a *method* mark: the right approach, even if the number is wrong.
- **A1** an *answer* mark, and it usually needs its M mark first.
- **C1** a working mark on the way to the answer.
- // separates answers the examiner accepts equally.
- **ecf** = error carried forward: a later part is marked on your own earlier answer.
- **owtte** = "or words to that effect" – the wording need not match.

Question 9

9701/42 N25 ▪ Q9 ▪ 14 marks

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

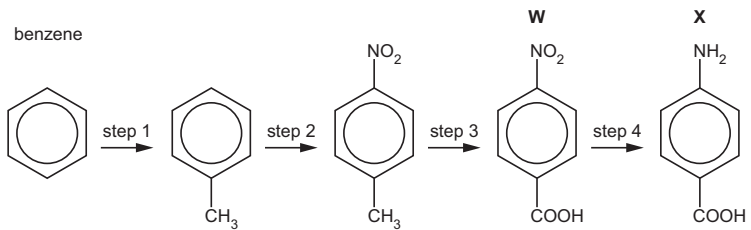


Fig. 9.1

(a) Describe the bonding in benzene, C_6H_6.

Question 9

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.

Question 9

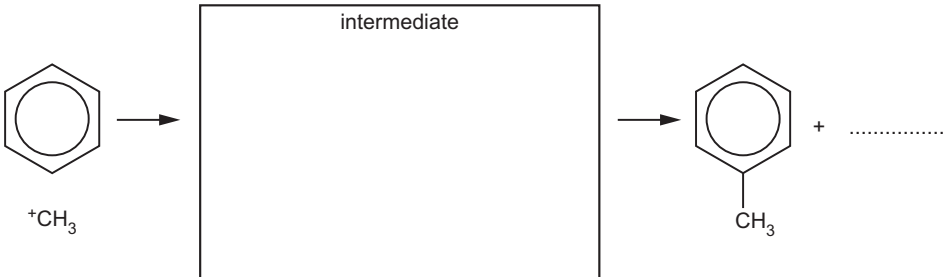
(b) Describe the reagents and conditions required for step 1 in Fig. 9.1.

Question 9

(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.



Question 9

Question 9

Fig. 9.2

[3]

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

Question 9

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

Question 9

(f) Name compound **W**.

Question 9

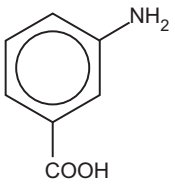
(g) The reagents commonly used for step 4 will **not** reduce the –COOH group.

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

Question 9

(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.

Question 9

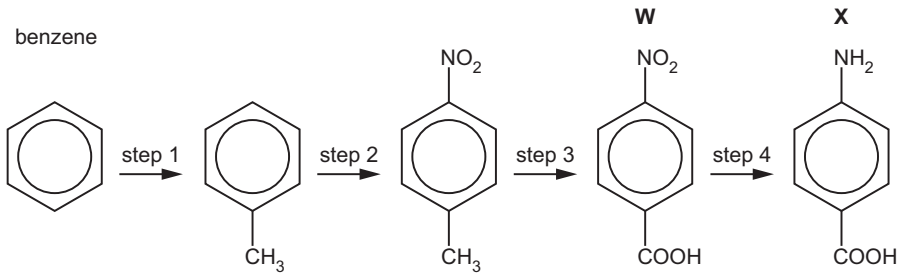


Fig. 9.1

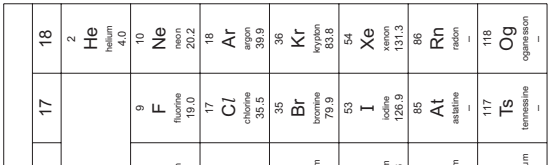
[Total: 14]

Important values, constants and standards

Question 9

Question 9

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



able of Elements

roup

			13	14	15	16
			5 B boron 10.8	6 C carbon 12.0	7 N nitrogen 14.0	8 O oxyger 16.0
			13 Al aluminium 27.0	14 Si silicon 28.1	15 P phosphorus 31.0	16 S sulfur 32.1
10	11	12				
28 Ni nickel 58.7	29 Cu copper 63.5	30 Zn zinc 65.4	31 Ga gallium 69.7	32 Ge germanium 72.6	33 As arsenic 74.9	34 Se seleniu 79.0
46 Pd palladium 106.4	47 Ag silver 107.9	48 Cd cadmium 112.4	49 In indium 114.8	50 Sn tin 118.7	51 Sb antimony 121.8	52 Te telluriu 127.6
78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.6	81 Tl thallium 204.4	82 Pb lead 207.2	83 Bi bismuth 209.0	84 Po poloniu –
110 Ds darmstadtium –	111 Rg roentgenium –	112 Cn copernicium –	113 Nh nihonium –	114 Fl flerovium –	115 Mc moscovium –	116 Lv livermoriu –

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 ytterbiu 173.1
96 Cm curium –	97 Bk berkelium –	98 Cf californium –	99 Es einsteinium –	100 Fm fermium –	101 Md mendelevium –	102 No nobeliu –

The Periodic T

G

1
H
hydrogen
1.0

Key

atomic number
atomic symbol
name
relative atomic mass

3	4	5	6	7	8	9
21	22	23	24	25	26	27
Sc	Ti	V	Cr	Mn	Fe	Co
scandium	titanium	vanadium	chromium	manganese	iron	cobalt
45.0	47.9	50.9	52.0	54.9	55.8	58.9
39	40	41	42	43	44	45
Y	Zr	Nb	Mo	Tc	Ru	Rh
yttrium	zirconium	niobium	molybdenum	technetium	ruthenium	rhodium
88.9	91.2	92.9	95.9	–	101.1	102.9
57–71	72	73	74	75	76	77
lanthanoids	Hf	Ta	W	Re	Os	Ir
	hafnium	tantalum	tungsten	rhenium	osmium	iridium
	178.5	180.9	183.8	186.2	190.2	192.2
89–103	104	105	106	107	108	109
actinoids	Rf	Db	Sg	Bh	Hs	Mt
	rutherfordium	dubnium	seaborgium	bohrium	hassium	meitnerium
	–	–	–	–	–	–

57	58	59	60	61	62	63
La	Ce	Pr	Nd	Pm	Sm	Eu
lanthanum	cerium	praseodymium	neodymium	promethium	samarium	europium
138.9	140.1	140.9	144.2	–	150.4	152.0
89	90	91	92	93	94	95
Ac	Th	Pa	U	Np	Pu	Am
actinium	thorium	protactinium	uranium	neptunium	plutonium	americium
–	232.0	231.0	238.0	–	–	–

1	2
3 Li lithium 6.9	4 Be beryllium 9.0
11 Na sodium 23.0	12 Mg magnesium 24.3
19 K potassium 39.1	20 Ca calcium 40.1
37 Rb rubidium 85.5	38 Sr strontium 87.6
55 Cs caesium 132.9	56 Ba barium 137.3
87 Fr francium –	88 Ra radium –

lanthanoids

actinoids

Solution 9

(a) Mark scheme

- ▪
- all C atoms are sp2 hybridised
- ▪
- bonds between C atoms are σ and π
- ▪
- C–C σ bonds are formed by overlap of sp2 hybrid orbitals
- ▪
- C–C π bonds are formed by overlap of p orbitals

Solution 9

- ▪
- bonds between C and H atoms are σ
- ▪
- C–H bonds are formed by overlap of sp2 hybrid orbitals and s orbitals
- Any two [1], any four [2], all six [3]
- 3
- 9701/42
- October/November 2025

Solution 9

(b)

Mark scheme

- CH3Cl and Al Cl 3/1

Solution 9

(c)

Mark scheme

- M1: curly arrow from within hexagon towards +C
- M2: intermediate, usual rules for horseshoe and + charge
- M3: curly arrow from C–H bond into ring AND H+ product
- 3

Solution 9

(d)

Mark scheme

- M1: HNO3 AND H2SO4
- M2: concentrated AND 25 °C T 60 °C
- 2

Solution 9

(e)

Mark scheme

- alkaline KMnO4
- 1

Solution 9

(f)

Mark scheme

- 4-nitrobenzoic acid
- 1

Solution 9

(g)

Mark scheme

- (hot) concentrated HCl and Sn
- 1

Solution 9

(h)

Mark scheme

- M1: perform step 3 before step 2 OR perform step 2 before step 1
- M2: COOH is 3-directing OR NO2 is 3-directing
- 2

Question 5

9701/44 N25 ▪ Q5 ▪ 13 marks

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.

Question 5

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

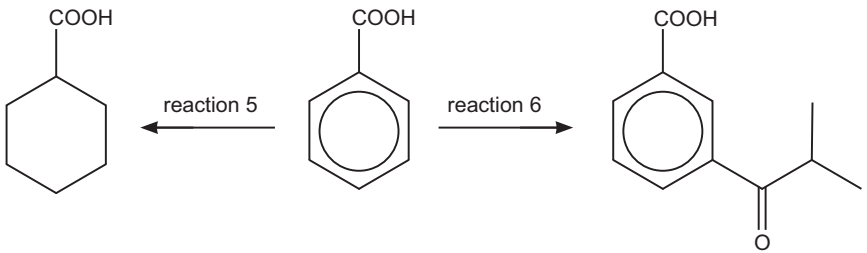


Fig. 5.1

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

Question 5

Question 5

[2]

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

Question 5

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

(i) Describe the directing effect of the $–CH_2CH_3$ group.

Explain your answer.

Question 5

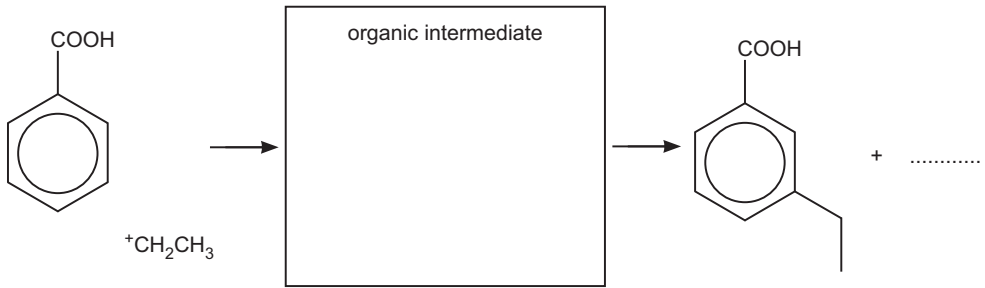
(ii) The alkylation of arenes uses a mixture of CH_3CH_2Br and $FeBr_3$ to generate the $CH_3CH_2^+$ electrophile.

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

Question 5

(iii) Complete the mechanism in Fig. 5.2.

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



Question 5

Fig. 5.2

Question 5

[3]

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

Question 5

[Total: 13]

Solution 5

(a) Mark scheme

- M1 and M2: any two [1], all three [2]
- ▪
- (hexagonal ring) planar / (trigonal) planar
- ▪
- 120o
- ▪
- sp2 hybridised

Solution 5

- M3: p orbitals overlap sideways / laterally (with each other above and below the ring) forming π bonds
- M4: σ bonds form when sp2 / hybridised orbitals overlap end-on-end / head on
- 4

Solution 5

(b)(i)

Mark scheme

- M1: (reaction 5)
- Pt / Ni + H2 (+ heat)
- M2: (reaction 6)
- (CH3)2CHCOCl + Al Cl 3 (+ heat)
- 2

Solution 5

(b)(ii)

Mark scheme

- reduction / hydrogenation
- 1

Solution 5

(c)(i)

Mark scheme

- (CH2CH3 group) directs to 2-, 4- (and 6-) positions AND due to being an electron donating group
- 1

(c)(ii)

Mark scheme

- CH3CH2Br + FeBr3 → CH3CH2+ + FeBr4–
- 1

Solution 5

(c)(iii)

Mark scheme

- M1: curly arrow from inside / touching the hexagon to (CH2) group / C+ charge
- M2: structure of the intermediate
- M3: curly arrow from C-H bond into / onto the ring AND formation / loss of H+
- 3

Solution 5

(c)(iv)

Mark scheme

- H+ + FeBr4– → HBr + FeBr3
- 1
- organic intermediate
- 9701/44
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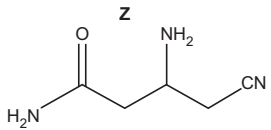
Question 6

9701/44 N25 ▪ Q6 ▪ 9 marks

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

Z



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

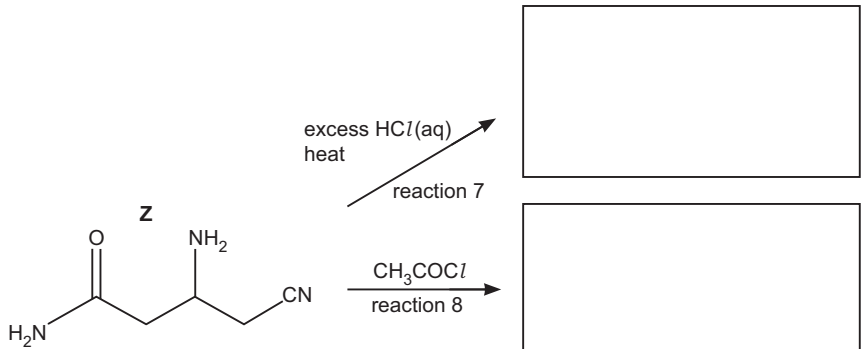
Table 6.1

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

Question 6

[1]

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



Question 6

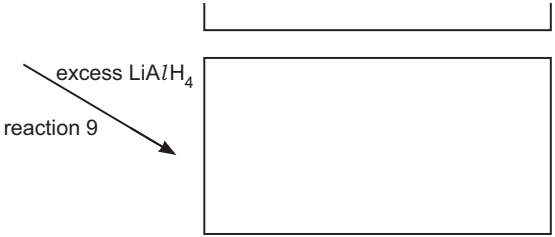


Fig. 6.1

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

Question 6

(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 D_2O 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**.

Question 6

(ii) The proton (^{1}H) NMR spectrum of **Z** in D_2O gives three peaks for the proton environments, labelled **a**, **b** and **c**, as shown on Fig. 6.2.

Z

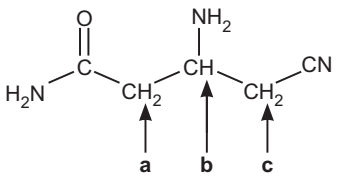


Fig. 6.2

Complete Table 6.2 for the proton (^{1}H) NMR spectrum of **Z** in D_2O.

Table 6.2

Question 6

Question 6

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	–C**H**$_3$, –C**H**$_2$–, >C**H**–	0.9–1.7
alkyl next to C=O	C**H**$_3$–C=O, –C**H**$_2$–C=O, >C**H**–C=O	2.2–3.0
alkyl next to nitrile	–C**H**$_2$–CN	2.0–3.0

Question 6

alkyl next to nitrile	CH_2 CN	2.0 3.0

Question 6

alkyl next to electronegative atom	C**H**$_3$–O, –C**H**$_2$–O, –C**H**$_2$–N	3.2–4.0
attached to alkene	=C**H**R	4.5–6.0
alkyl amine	R–N**H**–	1.0–5.0
amide	RCON**H**R	5.0–12.0

[Total: 9]

Solution 6

(a)

Mark scheme

- sp $= 1$ AND sp2 $= 1$ AND sp3 $= 3/1$

Solution 6

(b)(i)

Mark scheme

- acid-base / neutralisation AND hydrolysis
- 1

(b)(ii)

Mark scheme

- any two * [1], any three * [2], any five * [3], all six * [4]
- 4

Solution 6

(c)(i)

Mark scheme

- five / 5/1

Solution 6

(c)(ii) Mark scheme

- proton environment
- a
- b
- c
- name of splitting pattern
- doublet
- multiplet
- doublet

Solution 6

- chemical shift range,
- δ / ppm
- 2.2–3.0
- 3.2– 4.0
- 2.0–3.0
- any three [1], all six [2]
- 2
- reaction 7
- reaction 8
- reaction 9

Solution 6

- *
- *
- *
- *
- *
- *
- *
- *
- 9701/44
- October/November 2025