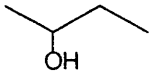
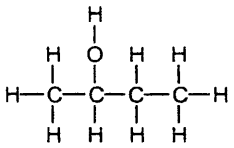
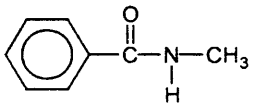
Marking structures in organic chemistry

When a structure is asked for, there must be sufficient detail using conventional carbon skeleton and functional group formulae (e.g. CH_3, C_2H_5, OH, COOH, $COOCH_3$) to unambiguously define the arrangement of the atoms. (E.g. C_3H_7 would not be sufficient).

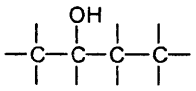
If not specified by the question, this may be given as either:

- a **structural formula** – e.g. $CH_3CH(OH)C_2H_5$,
- a **skeletal formula** – e.g.  ,
- a **displayed formula** – e.g. 

or as a hybrid of these – e.g. 

The following errors should be penalised – although each one only loses a maximum of one mark on the paper:

- clearly connecting a functional group by the wrong atom
- showing only 'sticks' instead of hydrogen atoms –

e.g. 

Benzene rings may be represented as  *as well as*  *in any of the types of formula above.*

1 (a) (i) ethanal ✓ **[1]**

(ii) aldehyde / carbonyl ✓ **[1]**

(iii) CH_3CH_2OH / C_2H_5OH ✓

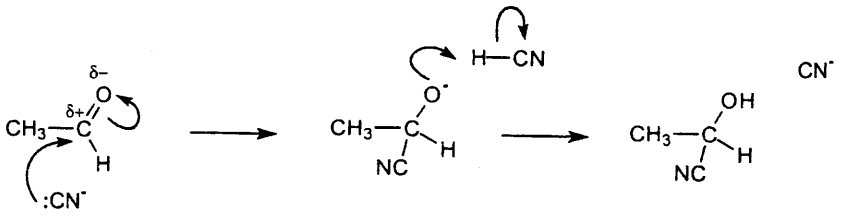
CH_3COO^- / CH_3COOAg / CH_3COOH ✓

allow displayed formulae, but penalise poor connections to the OH, sticks etc **[2]**

(b) (i) (nucleophile/CN^-) is an electron/lone pair donor ✓ **ESSENTIAL MARK**

then look for the following points:

in the diagram ...	**or a written alternative ...**	
CN^-	the nucleophile is CN^-	✓
curly arrow clearly starts from a lone pair drawn on the C	the electron/lone pair is donated from the C of the CN^-	✓
curly arrow towards $C^{\delta+}$ and breaking C=O	(nucleophile/ CN^-) is attracted to an electron deficient carbon	✓
correct structure of the intermediate	(nucleophile/ CN^-) forms a covalent/dative bond (to the carbon)	✓
correct structure of the product	HCN is added	✓



ANY 4 out of **5** **[5]**

(ii) HCN / KCN / CN^- is toxic / **AW**

NOT dangerous or explosive **[1]**

(iii) Yes, because ...
(the product) has a chiral centre/carbon ✓
four different groups around the carbon ✓
assymetric ✓
cannot be superimposed on its mirror image ✓

NOT "four different atoms" or "molecules"

allow ecf from b(i)

ANY 2 out of **4** **[2]**

[Total: 12]

2 (a) (i) $CH_3CHClCH_3$ ✓ allow any formula that is unambiguously 2-chloropropane **[1]**

(ii) $CH_3CHClCH_3 + C_6H_6 \longrightarrow C_6H_5CH(CH_3)_2 + HCl$ ✓ **[1]**

(iii) halogen carrier ✓ **[1]**

(b) (i) peaks identified
peak **X** – CH_3 (protons) ✓
peak **Y** – CH (proton) ✓
peak **Z** – benzene ring (protons) ✓

3 identification marks

reasoning from δ value ... for each, either:
- quotes a δ value for the peak **and** refers explicitly to the Data Sheet /or
- quotes the relevant functional group in the Data Sheet (eg R-CH_3 for X) /or
- quotes exactly the relevant Data Sheet range, ie (0.7–1.6 for X)
  (2.3 – 2.7 for Y)
  (7.1 – 7.7 for Z) ✓✓✓

ignore any attempts to reason from the splitting here, but look out for credit to parts (ii) and (iii) if not given below

3 reasoning marks **[6]**

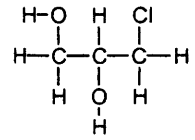
(ii) 1 proton / CH/ 'n' = 1 (using the n+1 rule) ✓

on the neighbouring/adjacent carbon ✓ **[2]**

(iii) the CH_3 protons are all equivalent/in the same (chemical) environment / there are six protons adjacent to the CH ✓ **[1]**

[Total: 12]

3 (a) (i)



the correct compound .... ✓

shown as a correctly displayed formula ✓ **[2]**

(ii) yes, because there are four different groups around the central carbon ✓
(or ecf on the structure given in (i)) **AW**

allow asymmetric / non-superimposable on its mirror image **[1]**

(b) infra-red/i.r. (spectroscopy) ✓
peak/absorption at 3230 - 3550 (cm^{-1}) ✓

n.m.r. (spectroscopy) ✓
peak at 3.5–5.5 (ppm) ... ✓
... which disappears in D_2O ✓

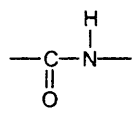
Quality of Written Communication
mark for good organisation / a logical response and technical terms, using at least **two** of the following words:
infra-red, nuclear magnetic resonance, spectroscopy, wavenumber, cm^{-1}, chemical shift, ppm) ✓ **[6]**

(c) (i) dil/conc/(aq) HCl
or dil/(aq) H_2SO_4 /H^+/acid
or dil/conc/(aq) OH^-/alkali/NaOH etc ✓

if a formula given, there must be some indication that it is aqueous

allow an enzyme as long as aq **[1]**

(ii)



✓ **[1]**

(iii) amino acids ✓

allow peptides **[1]**

[Total: 12]

4 (a) carboxylic acid / phenol / amino acid / named example or correct formula ✓

NOT 'HX' or any inorganic acid

equation to give the correct negative ion ✓
eg $CH_3COOH \rightleftharpoons CH_3COO^- + H^+$
/ $CH_3COOH + H_2O \rightleftharpoons CH_3COO^- + H_3O^+$

allow ecf on the formula or an inorganic acid from above as long as donation of H^+ shown **[2]**

(b) (i) $C_6H_5NH_2 + H_2O \rightleftharpoons C_6H_5NH_3^+ + OH^-$ ✓

do not penalise a correct equation using H^+ or another acid **[1]**

(ii) (base, phenylamine, ethylamine) accepts H^+ ✓ / donates lone pair

allow **AW** throughout

(uses the) lone pair on the nitrogen ✓

(or shown on a diagram)

the lone pair (in phenylamine) is delocalised /interacts with the delocalised/π electrons in the ring
or
inductive effect pulls electrons (from the nitrogen)
ora ✓

It must be clear which way the electrons are going" **[3]**

(c) amino acid / $RCH(NH_2)COOH$ / named example or correct formula ✓

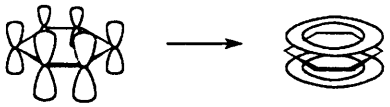
do not allow non-organic acids for the first mark, but give ecf on good explanation

contains both carboxylic acid/COOH and basic amine/NH_2 groups ✓

allow any explanation describing acidity and basicity eg "can donate and accept H^+") **[2]**

[Total: 8]

5 (a) planar molecule (or shown in diagram) ... ✓



p-orbitals (or shown in diagram) ✓
... overlap (or shown in a diagram) ✓

(p-orbital ovelap forms) π-bonds ✓
electrons are delocalised ✓
C-C bonds are all the same length ✓

ANY 5 out of **6**

Quality of Written Communication
mark for spelling, punctuation and grammar. Look for at least two sentences with legible text, accurate spelling, grammar and punctuation, so the meaning is clear ✓ **[6]**

(b) (i) $C_6H_5CHBrCH_2Br$ ✓ **[1]**

(ii) phenylethene has a double bond ✓

benzene (π) electrons are:
spread out / delocalised / lower electron density
✓ **ora** for **2** marks

then either ...
so the bromine molecule gets less polarised / needs the catalyst to help polarise it ... ✓

and the bromine/electrophile is less strongly attracted (to the π electrons) ✓
ora and AW for **2** marks

or ...
(delocalised (π) electrons make) benzene stable ... ✓

so more energy is needed (to overcome it) / higher E_a / it is not easily disrupted ✓
ora and AW for **2** marks

TOTAL 2 + 2 marks **[4]**

(c) (to make) poly(phenylethene) / polymers / plastics / a named use of poly(phenylethene) ✓
eg packaging, insulation, toys, moulded casings etc **[1]**

[Total: 12]

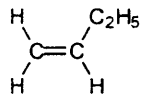
6 (a) 184 [1]

(b) (i) **identification of the compounds ...**
any type of formula that unambiguously identifies the compound – eg

B

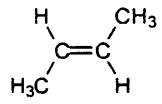
$CH_3CHICH_2CH_3$ ✓

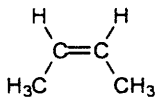
C



✓

D and **E**



and


✓✓

F

$CH_3CH_2CH_2CH_3$ ✓

5 marks

reasoning ...
H can be taken from either carbon 1 or carbon 3 ✓ **AW**

D and **E** are cis-trans/geometric (isomers) ✓

double bond does not rotate ✓

explanation why but-2-ene gives cis/trans isomers or why but-1-ene doesn't ✓

ANY 3 out of **4** marks [8]

(ii) addition / hydrogenation / reduction ✓ [1]

[Total: 10]

7 (a) (i) tin/iron ✓

hydrochloric acid / HCl ✓

allow $LiAlH_4$ ✓ anyhydrous/ether ✓

[2]

(ii) M_r of $C_6H_5NO_2$ = **123**(.0) ✓
M_r of $C_6H_5NH_2$ = **93**(.0) ✓

(use of correct M_r s get **2** marks)

theoretical mass of $C_6H_5NH_2$ = **7.56**(g) /ecf
/ moles of $C_6H_5NH_2$ = **0.08(13)** /ecf ✓

answer in the range **89.8-90.0**(%) /ecf 3 sf ✓

(correct answer gets **2** more marks)

answer in the range **87-92%** due to rounding errors and/or with sig figs ≠ 3 gets **3** marks max

[4]

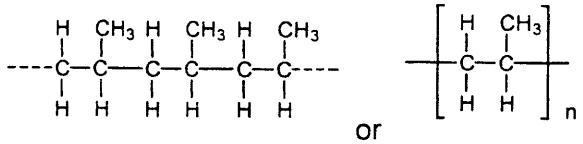
(b) sodium nitrite + (hydrochloric) acid
/ nitrous acid / HNO_2 ✓✓

< 10°C ✓

[3]

[Total: 9]

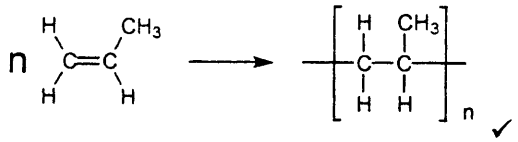
8 (a) (i) a correct structure for poly(propene), eg



or ✓

bonds must extend outside any brackets

equation showing 'n' monomers



✓

[2]

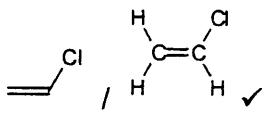
(ii) addition:
monomer has C=C double bond / is an alkene / double bond breaks/ no (other) substance lost ✓

NOT just "monomer has a double bond"

condensation:
water / small molecule lost ✓

[2]

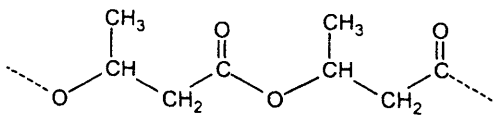
(b)



✓

[1]

(c) (i)



at least one correct ester link ✓
rest of the structure and repeat also correct ✓

allow a break in the repeat at any point

[2]

(ii) H reacts with NaOH / poly(propene) does not ✓

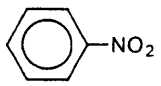
H is an ester / is polar ... ✓
will be hydrolysed by NaOH ✓
poly(propene) is non-polar ✓

"hydrolysed by NaOH" gets the reacts with NaOH mark as well

ANY 3 out of **4** marks

[3]

[Total: 10]

9 (a)  / $C_6H_5NO_2$ ✓

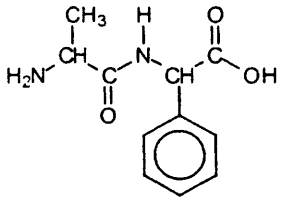
allow poly-nitrated benzene in any positions

[1]

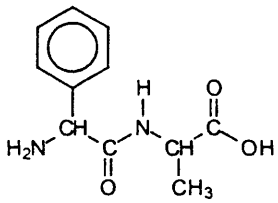
(b) CH_3COOH ✓ CH_3OH ✓

[2]

(c) two structures made by joining the amino acids



either way round – eg



peptide bond in one structure ✓

two dipeptides with R groups swapped ✓

allow H_2O ✓ and one correct dipeptide ✓ as an alternative answer

[2]

[Total: 5]