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, COOCH₃) 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. CH₃CH(OH)C₂H₅,
- a **skeletal formula** e.g.

H H O H H H-C-C-C-C-H

• a displayed formula - e.g

C-N-CH3

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 –

Benzene rings may be represented as of the types of formula above.

as well as

¹ Note that in organic chemistry a candidate may identify a compound by name and formula. If one of these is wrong then the mark is not awarded as this is a contradictory answer.

1 (a) (i)

[1]

(ii) $C_6H_6 + CH_3CI \longrightarrow C_6H_5CH_3 + HCI \checkmark$

[1]

(iii) iron / aluminium chloride / iron(III)chloride etc Fe / AlCl₃/ FeCl₃ ✓

[1]

(iv) any polymethylated benzene ring ✓

name ✓ eg 1,2-dimethylbenzene/ 1,4-dimethylbenzene

[2]

(b) (i)

brominated phenol ✓ 2,4,6 substituted ✓ balancing ✓

[3]

(ii)

phenoxide ✓ balancing ✓

[2]

[1]

(c) any general use that contains phenois - eg

antiseptics / disinfectants /dyes / plastics /pharmaceuticals / pesticides/explosives 🗸

[Total: 11

2 (a) (i) (trigonal) pyramidal ✓

[1]

(ii) tetrahedral ✓

[1]

(iii) trigonal (planar) ✓

[1]

(b) (i) H₃N⁺CH₂COOH ✓

[1]

(ii) NH₂CH₂COO ⁻ ✓

[1]

(c) (i) H⁺ / acid / HCI / H₂SO₄ / OH ⁻ / alkali ✓ /heat / reflux ✓

(or use of an enzyme at 37°ish)

[2]

(ii) hydrolysis ✓

[1]

(d) (i) carbon with four different / distinguishable groups attached ✓

(or carbon / part of the molecule / atom which is assymetric / non-superimposible on its mirror image)

[1]

(ii)

one structure of alanine with at least one 3-d bond ✓ two optical isomers / reflections of a 3-d structure ✓

[2]

(iii) one stereoisomer ✓

natural /from a living system / made by enzymes etc ✓

[2]

[Total: 13]

3 (a) ester ✓ (primary) amine ✓

[2]

(b) (i) C₈H₉NO₂ ✓

[1]

(ii) M_r of A = 151 (or ecf from (i) \checkmark

moles A = 0.100g/151 = 0.000662conc. A = 0.000662/0.330dm³ = 0.002 /0.0020 (ecf from a wrong M_r) \checkmark

[2]

(c) (i) peaks identified

peak X – benzene ring protons ✓ peak Y – CH₂ protons ✓ peak Z – CH₃ protons ✓

3 identification marks

reasoning from δ value ... for each, either:

- quotes the relevant functional group in the Data Sheet (eg –O-CH₂-R) /or
- quotes the relevant Data Sheet range (eg 3.3-4.3) / or
- from first principles using the expected deshielding to assign the peaks

√√、

reasoning from the splitting pattern ...

- Y peak is a quadruplet/1:3:3:1 etc this is due to 3 neighbours / adjacent to a CH₃ ✓
- Z peak is a triplet / 1:2:1 etc this is due to 2 neighbours /adjacent to a CH₂ ✓

ANY 3 out of 5 reasoning marks [6]

(ii) peak at 1700cm⁻¹ and/or at 1280cm⁻¹ marked ✓

[1]

[Total: 12]

4 (a) (i) reagents conc H₂SO₄ + HNO₃ ✓

electrophile
$$NO_2^+\checkmark$$

 $H_2SO_4^- + HNO_3^- \longrightarrow HSO_4^- + H_2O_+ NO_2^+/$
 $2H_2SO_4^- + HNO_3^- \longrightarrow 2HSO_4^- + H_3O^+ + NO_2^+\checkmark$

mechanism

curly arrow from benzene π -bond to electrophile \checkmark correct intermediate (ecf on electrophile formula) \checkmark curly arrow from C-H bond to π -bond and H $^+$ formed \checkmark

overall equation

$$C_6H_6 + HNO_3 \longrightarrow C_6H_5NO_2 + H_2O \checkmark$$

ANY 6 out of **7** [6]

(ii) NO₂⁺ accepts an electron pair ✓ H is replaced / substituted by NO₂ ✓

[2]

(b) two peaks ✓ peak at/between 2.3-2.7 ✓ peak at/between 7.1-7.7 ✓

[3]

[Total: 11]

5 (a)

any unambiguous type of formula ✓✓✓✓

[4]

(b) (i) butan-1-ol gives butanal /butanoic acid / an aldehyde / a carboxylic acid butan-2-ol gives butanone / a ketone
 2-methylpropan-2-ol gives no reaction ✓✓✓

3 marks for the alcohol reactions

D is methylpropan-1-ol ✓ E is methylpropanoic acid ✓ ✓ (where any carboxylic acid for E gets the first mark)

> 3 marks for identifying D and E Any 5 out of 6

Quality of Written Communication

information is organised clearly and coherently using at least **two** specialist terms not mentioned in the question (eg correct names of compounds, primary, secondary, aldehyde, ketone, oxidised etc.) ✓

[6]

(ii)
$$(CH_3)_2CHCOOH + C_2H_5OH \longrightarrow (CH_3)_2CHCOOC_2H_5 + H_2O / C_4H_8O_2 + C_2H_6O \longrightarrow C_6H_{12}O_2 + H_2O / ecf from (i) \checkmark$$

[1]

wnere

-OH ✓ -COO - / COO - Na - / COONa ✓

[Total: 13

6 (a) (i) nucleophilic addition ✓

CN ⁻ ✓

both curly arrows / arrow from nucleophile and dipole ✓

both curly arrows ✓

intermediate ✓

ANY 4 out of 6 [4]

... and X 🗸

(ii) HCI / H₂SO₄ / H⁴ / acid ✓ hydrolysis ✓ [2]

(iii) OH
CH₃—C
COOH
H
(1]

(b) 1 doublet and 1 quadruplet / 1:3:3:1 and 1:1 ✓ correct reason for at least one peak ✓ (eg 1;3:3;1 due to 3 neighbours / next to CH₃ / use of n+1 rule) [2]

(iii) OH (2]

[Total: 13]

7 (a) L:

M:

[3]

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

[2]

(c) condensation ✓ loss of water / small molecule ✓

[2]

(d) fibres / clothing / bottles etc ✓

[1]

[Total: 8]

8 to detect the presence of C=O ...

2,4-dinitrophenylhydrazine / 2,4-DNPH ✓ red/orange/yellow ppt/solid/crystals ✓

or

i.r. spectrum ✓ has peak at 1680-1750 cm⁻¹ ✓

2 marks

to confirm it is a ketone not an aldehyde ...

Tollens' reagent /(acidified) K₂Cr₂O₇ ✓ aldehyde: silver mirror / green colour ✓ ketone: no silver mirror / no green colour ✓

or

n.m.r. spectrum ✓ aldehyde: peak at 9.5-10 ✓ ketone: no peak at 9.5-10 ✓

3 marks

a chemical method to identify the ketone ...

use the product / solid / ppt from 2,4-DNPH / 2,4-dinitrophenylhydrazine ✓ (re)crystallise / purify (the product) ✓ measure the melting point ✓ compare with known compounds / data book ✓

4 marks

ANY 8 marks out of 9 [8]

Quality of Written Communication

at least two sentences with legible text, accurate spelling, grammar and punctuation, so the meaning is clear \checkmark

[1]

[Total: 9]