A-Level Chemistry

Hydrogen NMR

Mark Scheme

Time available: 62 minutes
Marks available: 59 marks

1. (a) Tick in carbonyl box only

1

(b) Peak at 2220-2260 cm^{-1} (for C≡N) disappears

If both C≡N disappears and N-H appears without wavenumbers scores 1

M1

Peak at 3300-3500 cm^{-1} (for N-H) appears

M2

Fingerprint region different

M3

(c) Integration ratio 2:2:3

If no link between delta value and oxygen and chlorine, then can award 1 mark for correct explanation of splitting of all 3 peaks

M1

Peak at 3.95 triplet (integration 2) Cl-CH_2 next to CH_2

M2

Peak at 3.65 triplet (integration 2) O-CH_2 next to CH_2

If no explanation of splitting, then can award 1 mark for 3 correct links between delta value and oxygen and chlorine M1

M3

Peak at 3.35 singlet (integration 3) O-CH_3 no adjacent H

M4

Structure CH_3-O-CH_2CH_2Cl

M5

[9]

2. (a)

1×AO1

1

(b) **S**

1

R

1

Q

1

(c) (Isomer **T**)

signals due to OH (alcohol) at 3230−3350 and C=O at 1680−1750

1

OH and C=O (functional groups) separated in molecule.

Allow not a carboxylic acid.

1

(Isomer U)

(only) signal for OH (alcohol) at 3230−3350

1

2 × OH groups present / diol / OH & cyclo(ether) structure.

Allow OH but not C=O.

1

(Isomer V)

signals due to OH (acid) at 2500−3000 (and C=O at 1680−1750)

carboxylic acid group / −COOH present.

1
1

(d) 2:2:2:3:3

Any order.

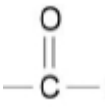
1

(e) (The quartet at δ=3.5 is for a CH_2 group) next to −**O**−**CH**$_2$ **OR** shifted significantly downfield by electronegative O

1

(is a quartet) because of an adjacent CH_3 group / couple with 3 adjacent protons

1

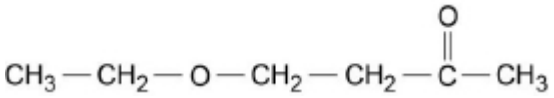
(singlet at δ=2.2 is for a CH_3 group) attached to  C**H**$_3$ **OR** shifted downfield by electronegative C=O

1

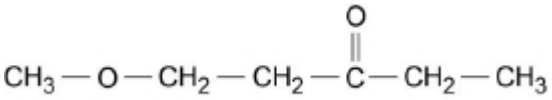
(is a singlet) because there are no adjacent protons / no coupling.

1

(f)



Allow 1 mark for:



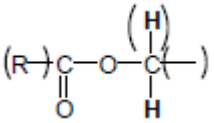
2

[17]

3. (a) M1 Ester **1**

If Ester 2, can score M3 only.

1

M2 peak at δ = 4.1 due to 

When marking M2 and M3, check any annotation of structures in the stem at the top of the page.

1

M3 (δ = 4.1 peak is) quartet as adjacent / next to / attached to CH_3

1

M4 Other spectrum quartet at δ = 2.1-2.6 (or value in this range)

1

(b) M1 Quaternary (alkyl) ammonium salt / bromide

1

M2 CH_3Br or bromomethane

Penalise contradictory formula and name.

1

M3 Excess (CH_3Br or bromomethane)

Mention of acid eg H_2SO_4 OR alkali eg NaOH loses both M2 and M3.

1

M4 Nucleophilic substitution

Can only score M3 if reagent correct.

Ignore alcohol or ethanol (conditions) or Temp.

1

(c)

	Bromine (penalise Br but mark on)	Acidified $KMnO_4$ (Penalise missing acid but mark on)

Wrong reagent = no marks.

If bromine colour stated it must be red, yellow, orange, brown or any combination, penalise wrong starting colour.

1

Benzene	no reaction / colour remains / no (visible) change	no reaction / colour remains / no (visible) change

Ignore 'clear', 'nothing'.

Allow colour fades slowly.

Allow 'nvc' for no visible change.

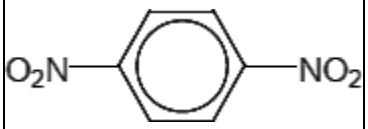
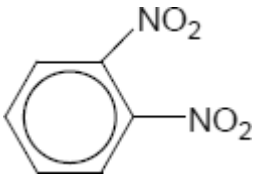
1

cyclohexene	(Bromine) decolourised	(Acidified $KMnO_4$) decolourised

1

[11]

4. (a)

F	G
	

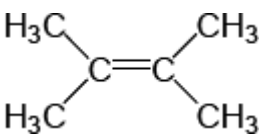
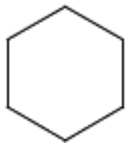
Penalize $-O_2N$ once

Penalise missing circle once

Don't penalise attempt at bonding in NO_2

1

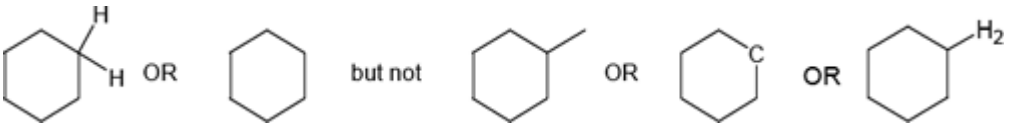
(b)

H	J
	

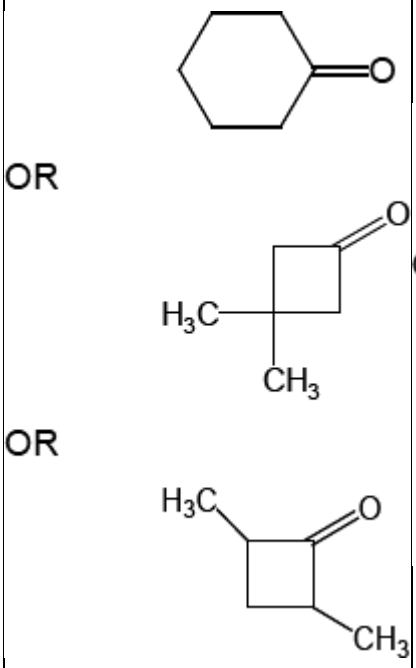
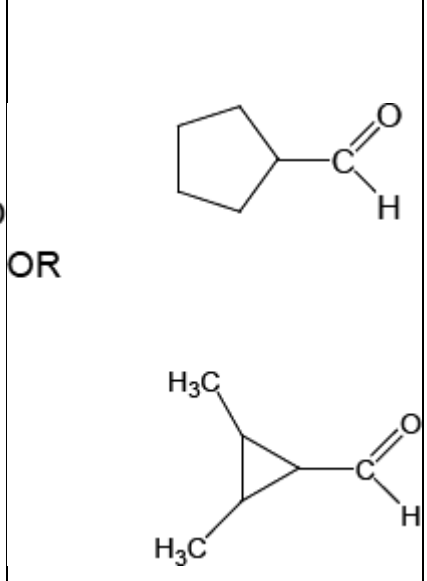
*If **both H** and **J** correct but reversed, award one mark*

1

A carbon in saturated ring structures should be shown as

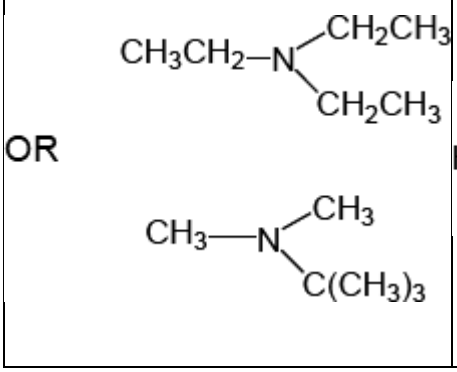
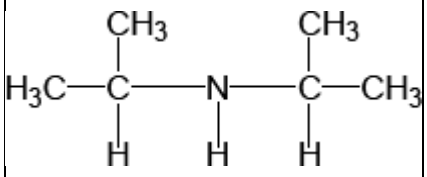


(c)

K	L
	

1

(d)

M	N
	

Allow C_2H_5 but

NOT allow C_4H_9 or C_3H_7

1

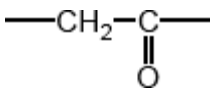
1

[8]

5. (a) OH alcohols

1

(b) (i) 2.6



Ignore any group on RHS

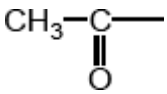
*Must clearly indicate relevant **two** H on a C next to C=O*

On LHS, penalise H or CH or CH_2 or CH_3

Ignore missing trailing bonds or attached R groups

1

(ii) 2.2



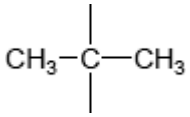
Ignore all groups on RHS

*Must clearly indicate relevant **three** H on C next to C=O*

Ignore missing trailing bonds or attached R group

1

(iii) 1.2



Or in words: two equivalent CH_3 groups

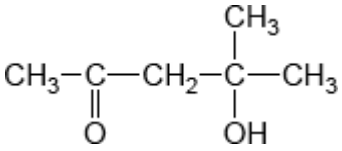
Must clearly indicate two equivalent methyl groups.

Penalise attached H

Ignore missing trailing bonds or attached R groups

1

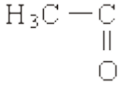
(iv)



1

[5]

6. (a) (i)



or $RCOCH_3$;

(or description in words)

(ignore trailing bonds)

1

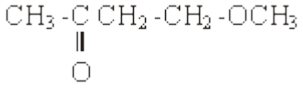
(ii) $H_3C—O$ or $ROCH_3$;

(allow 1 if both (i) and (ii) give CH_3- or H_3C– only)

1

(iii) CH_2CH_2 or two <u>adjacent</u> methylene groups;

1

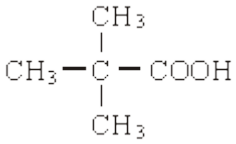
(iv) 

OR

$CH_3COCH_2CH_2OCH_3$;

1

(b) (i) OH <u>in acids</u> or (carboxylic) acid present

(ii) 

(c)

reagent	$K_2Cr_2O_7$ /H^+	$KMnO_4$ /H^+
Y	no reaction	no reaction
Z	orange to green or turns green	purple to colourless or turns colourless

5

[9]