Mark Scheme - C3.5 Instrumental Analysis

1 (a) (i) % H = 14.3 (1)

$$C : H = \frac{85.7}{12.0} : \frac{14.3}{1.01} = 7.14 : 14.16 \text{ (1)}$$

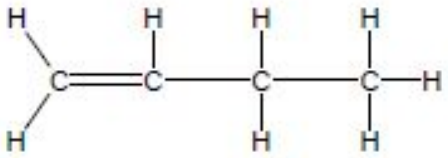
empirical formula = CH_2 (1) [3]

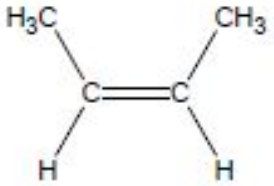
(ii) M_r = 42/ largest fragment has mass 42 (1)

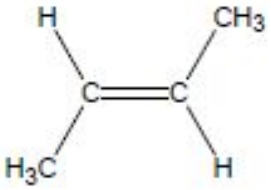
(CH_2 = 14) therefore molecular formula = C_3H_6 (1) [2]

(iii) CH_3 is present [1]

(b) 1 mark for each [3]

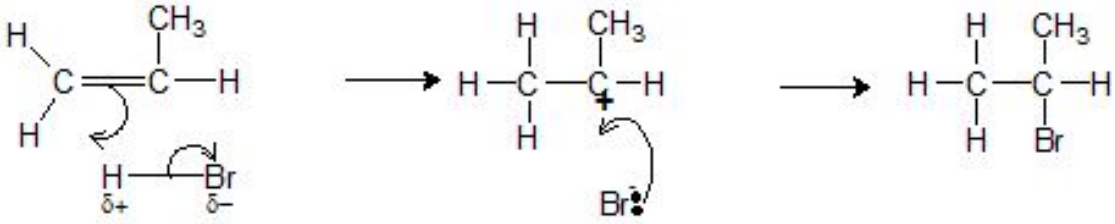






Total [9]

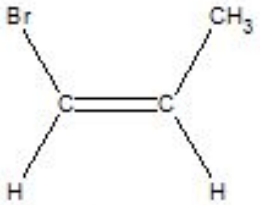
2 (a) (i) 1 mark for arrows in first diagram; 1 mark for arrow in second diagram; 1 mark for all charges



2 max if incorrect isomer given [3]

(ii) 2-bromopropane formed from a secondary carbocation (1)
Secondary carbocations are more stable than primary carbocations (1) [2]

(b) Empirical formula = C_3H_5Br (1)
Molecular formula = C_3H_5Br
(must show use of mass spectrum to gain this mark) (1)
Two molecular ion peaks as there are two isotopes of bromine (1)
Peaks at 15 = CH_3^+ and 41 = $C_3H_5^+$ (1)
550 cm^{-1} = C–Br 1630 cm^{-1} = C=C 3030cm^{-1} = C–H (1)
Molecule is:



(1) [6]

QWC: legibility of text, accuracy of spelling, punctuation and grammar, clarity of meaning [1]

Total [12]

3 (a) (i) Mass C = 1.79 × 12/44 = 0.488 (g) [1]

(ii) Mass O = 0.65 (g) ecf from part (i) [1]

(iii) C : H : O = 0.488/12 : 0.061/1 : 0.65/ 16 = 0.0407 : 0.061 : 0.0406 (1)

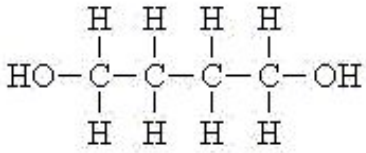
= 2:3:2 empirical formula is $C_2H_3O_2$ (1)

No ecf from incorrect ratios [2]

(iv) *Mr* of empirical formula = 59 so molecular formula is $C_4H_6O_4$ so **F** is acid 2/ molecular formula acid 1 is $C_5H_8O_2$ so empirical formula is not $C_2H_3O_2$ molecular formula acid 2 is $C_4H_6O_4$ so empirical formula is $C_2H_3O_2$ [1]

(v) Bromine turns from brown/red-brown to colourless for Acid 1 [1]

(vi)



[1]

(b) (i) *Mr* / molecular ion (is 46) [1]

(ii) CH_3 (present) [1]

(iii) OH (present) [1]

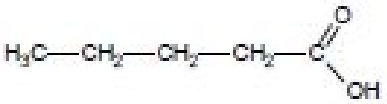
(c) Ethene to ethanol: steam (1)

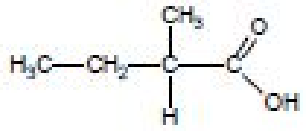
H_3PO_4 (catalyst) (1)

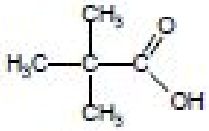
Ethanol to ethene: conc H_2SO_4/ Al_2O_3/ pumice (1)

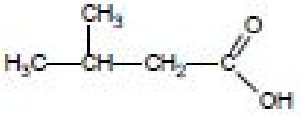
High temperature > 150°C for H_2SO_4
> 300°C for Al_2O_3/ pumice (1) [4]

Total [14]

4 (a) P is  (1)

Q is  (1)

R is  (1)

S is  (1)

[4]

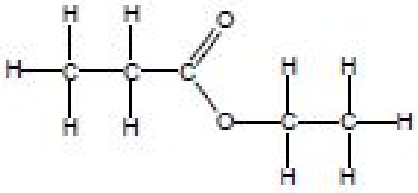
(b) (I) T neutral and sweet-smelling therefore an ester (1)

Infrared spectrum at 1750 cm^{-1} shows C=O and at 3000 cm^{-1} shows O–H therefore X is an acid (1)

Y is an alcohol, formed from ethanal must be ethanol (1)

5 carbons in ester therefore X must be propanoic acid (1)

Structure of T is

 (1)

(Maximum 4 marks) [4]

QWC Legibility of text; accuracy of spelling, punctuation and grammar, clarity of meaning (1)

Selection of a form and style of writing appropriate to purpose and to complexity of subject matter (1) [2]

(II) I Reagent to form Y is $NaBH_4$ / $LiAlH_4$ [1]

II Sulfuric acid acts as a catalyst / removes water so pushes equilibrium to right [1]

(c)

$CH_3(CH_2)$	0.1 to 2.0 ppm triplet (1)	
$(CH_3)CH_2O$	3.5 to 4.0 ppm quadruplet (1)	
CH_2CO	2.5 to 3.0 ppm singlet (1)	
CH_3CO	2.0 to 2.5 ppm singlet (1)	[4]

(d) Isomer P (1)

Only P can form hydrogen bonds between molecules (1)

Hydrogen bonds are the strongest intermolecular bonds / need more energy to break hydrogen bonds (1) [3]

QWC The information is organised clearly and coherently, using specialist vocabulary where appropriate [1]

Total [20]