

MEASUREMENT Core (SL & HL)

1. An unknown organic compound, X, was investigated using a variety of analytical techniques.

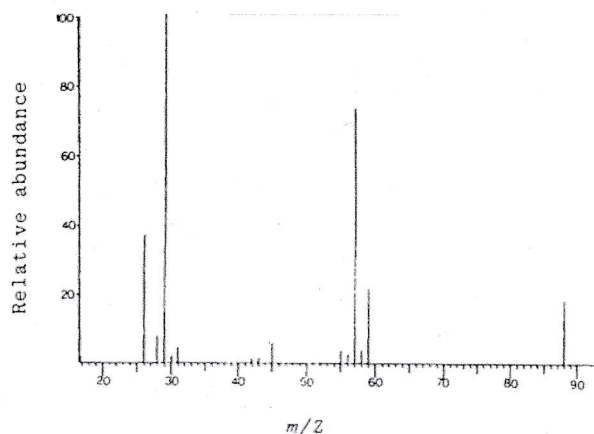
(a) Elemental analysis found that the compound had the following composition by mass:
54.5% carbon, 9.2% hydrogen and 36.3% oxygen.

(i) Determine the empirical formula of compound X.

[2]

$\frac{54.5}{12.01} = 4.537...$	$\frac{9.2}{1.01} = 9.108...$	$\frac{36.3}{16.00} = 2.268...$	✓
÷ by smallest	2	4	1
empirical formula is C_2H_4O ✓			

(b) The mass spectrum of compound X is shown below.



(i) Determine the mass of the molecular ion peak, and hence deduce the molecular formula for compound X.

[2]

88 ✓ C_2H_4O has mass of 44 $\frac{88}{44} = 2$

so molecular formula is $C_4H_8O_2$ ✓

(ii) Using section 28 of the data booklet, identify species responsible for peaks at $m/z = 29$ and 57.

[2]

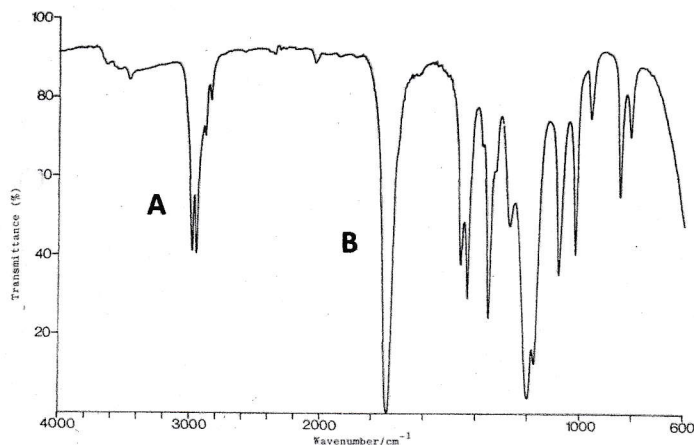
29: $[C_2H_5]^+$ ✓

57: $[C_2H_5CO]^+$ ✓

pendice missing + once only.

(allow alternatives - e.g. $[CHO]^+$ for 29.)

(c) The infrared (IR) spectrum of compound X is shown below.



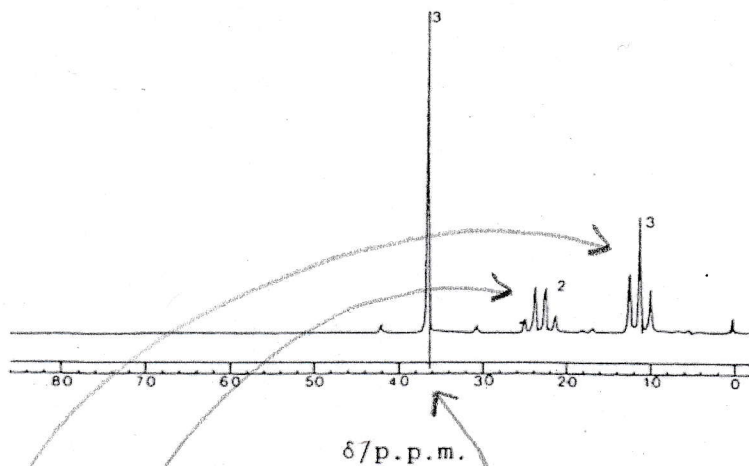
(i) Identify the bonds in the molecule causing the bands labelled A and B (using section 26 of the data booklet).

[2]

A: C-H ✓

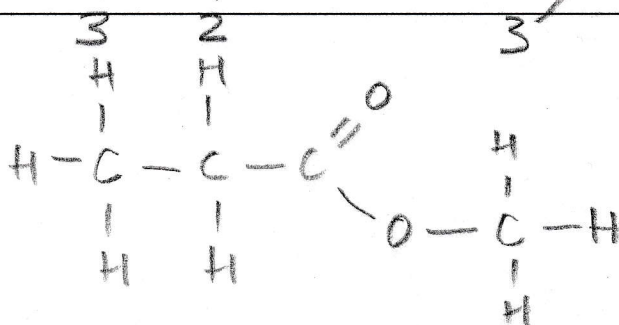
B: C=O ✓

(d) The $^1\text{H-NMR}$ spectrum of compound X is shown below:



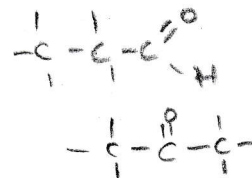
(i) Deduce the full structural formula of compound X using section 27 of the data booklet.

[1]



chemical shift data suggests methyl propanoate rather than ethyl ethanoate. ✓

2. Two isomers, propanal and propanone, have molecular formula C_3H_6O .



(a) State whether infrared (IR) spectroscopy could be used to distinguish between propanal and propanone. Explain your reasoning.

[1]

No, as IR shows the bonds present in the molecule
— and bonds are the same (in propanal & propanone)

(b) Using section 28 of the data booklet, identify the m/z of a species that might be found in the mass spectrum of **both** propanal and propanone.

[1]

15 / (CH_3^+) ✓ allow ions

(c) Using section 28 of the data booklet, identify the m/z of a species that might be found in the mass spectrum of propanal, but **not** in propanone.

[1]

29 / $(C_2H_5^+$ or $CHO^+)$ ✓ allow ions.

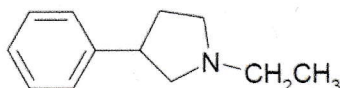
(d) Identify the number of hydrogen environments and hence the number of peaks in the 1H -NMR spectrum of propanal and propanone.

[2]

Propanal: 3 ✓
Propanone: 1 (molecule is symmetrical) ✓

3. Deduce the index of hydrogen deficiency for ethyne ($H-C\equiv C-H$) and for compound Y:

Compound Y



[2]

Ethyne: 2 (1 triple bond) ✓
Compound Y: 5 (2 rings & 3 double bonds) ✓

Total Marks 16 (24 minutes)