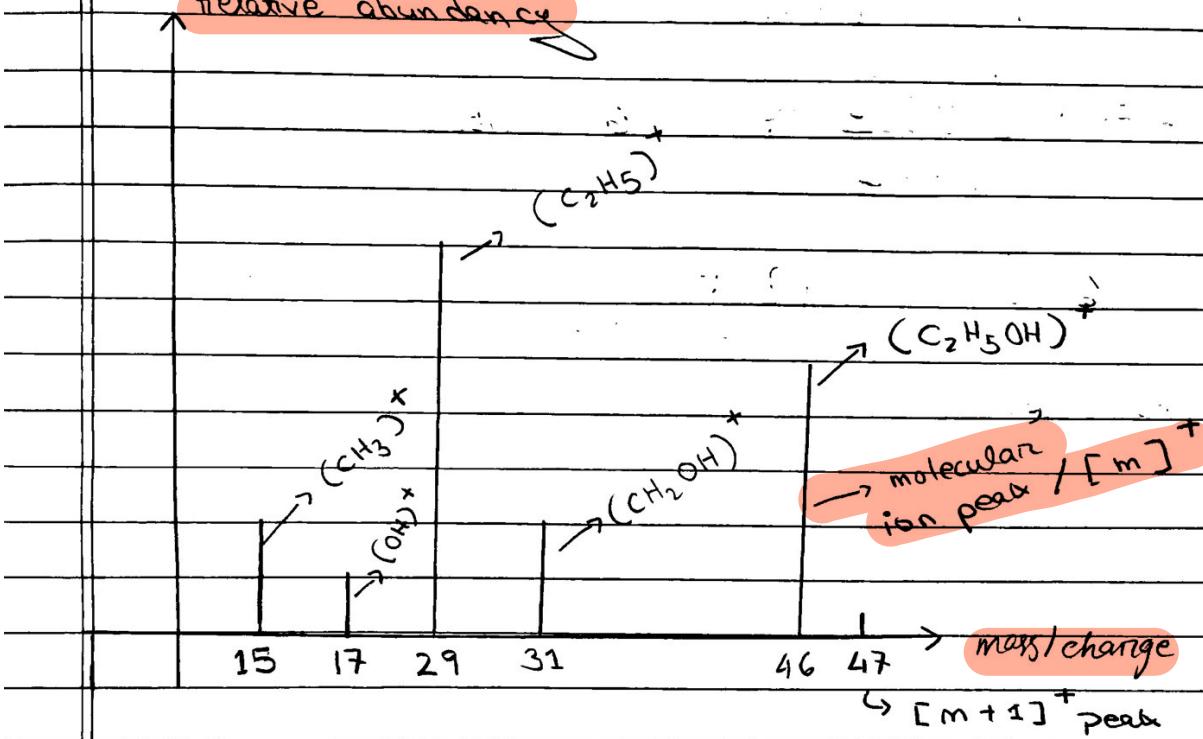


- Assumptions
(need confirmation)
- Raj bhaiya imp notes
- Stuff I added
(confirmed)

Mass Spectrometry

During Molecular fragmentation, mostly C-C single bond, C-N single bond and C-O^{single} bonds are broken down.

relative abundance



Used to identify unknown compound

The molecular ion peak is NOT always the highest peak; however it will always have a SIGNIFICANT height

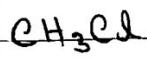
$$\hookrightarrow \text{no. of C atoms} = \frac{100}{1.1} \times \frac{[M+1] \text{ (R.A. / y-axis)}}{[M] \text{ (R.A. / y-axis)}}$$

A straight chain hydrocarbon has an $[m]^+$ at 84 mass/charge ratio, with a relative abundance of 62%, and an $[m+1]^+$ peak with a relative abundance of 4.1%. Name the hydrocarbon, given that it does not decolorise bromine.

$$\frac{100}{62} \times \frac{[m+1]}{[m]} = 6 \text{ carbon atoms}$$

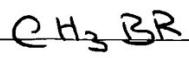


cyclohexane



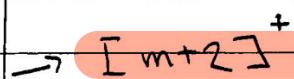
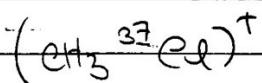
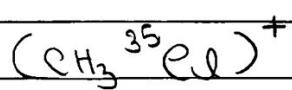
$$\text{CH}_3^{35}\text{Cl} = 50$$

$$\text{CH}_3^{37}\text{Cl} = 52$$

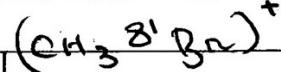
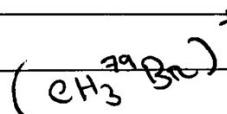


$$\text{CH}_3^{79}\text{Br} = 94$$

$$\text{CH}_3^{81}\text{Br} = 96$$



50 51 52



94 95 96

In case of $\text{Br} \text{ or } \text{M} : [\text{M}+2] = 1:1$

" " " Cl $[\text{M}] : [\text{M}+2] = 3:1$



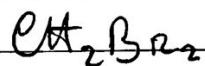
$$\text{CH}_2 \overset{35}{\text{Cd}} \overset{35}{\text{Cd}} = 84$$

$$\text{CH}_2 \overset{35}{\text{Cd}} \overset{37}{\text{Cd}} = 86$$

$$\text{CH}_2 \overset{37}{\text{Cd}} \overset{37}{\text{Cd}} = 88$$

$$[m] : [m+2] : [m+4]$$

$$9 : 6 : 1 \rightarrow \# (3x+y)^2 \\ = 9x^2 + 6xy + y^2$$



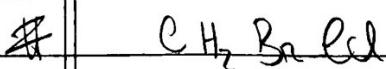
$$\text{CH}_2 \overset{79}{\text{Br}} \overset{79}{\text{Br}} = 172$$

$$\text{CH}_2 \overset{79}{\text{Br}} \overset{81}{\text{Br}} = 174$$

$$\text{CH}_2 \overset{81}{\text{Br}} \overset{81}{\text{Br}} = 176$$

$$[m] : [m+2] : [m+4]$$

$$1 : 2 : 1 \rightarrow \# (x+y)^1 \\ x^2 + 2xy + y^2$$



$$\text{CH}_2 \overset{79}{\text{Br}} \overset{35}{\text{Cd}}$$



$$\text{CH}_2^{79}\text{Br}^{35}\text{Cl} = 128$$

$$\begin{array}{l} \text{CH}_2^{81}\text{Br}^{35}\text{Cl} = 130 \\ \text{CH}_2^{79}\text{Br}^{37}\text{Cl} = 130 \end{array} \quad \left. \right\} \text{Will overlap to give one peak}$$

$$\text{CH}_2^{81}\text{Br}^{37}\text{Cl} = \cancel{130} \quad 132$$

→ (Infrared)

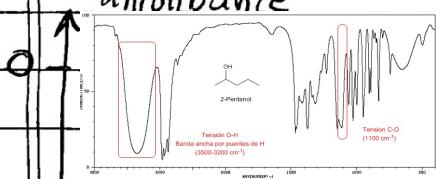
IR Spectroscopy

Transmittance %

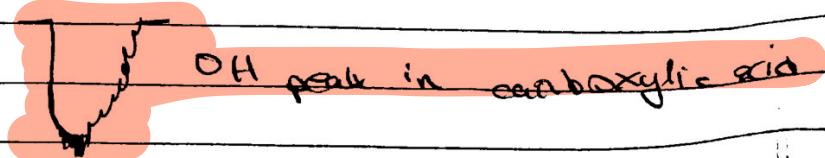


Wave Number = $\frac{1}{\lambda}$

The y-axis can also be absorbance, but then the scale will be flipped (from 100% to 0%), so the overall graph will be the same



OH peak in alcohol

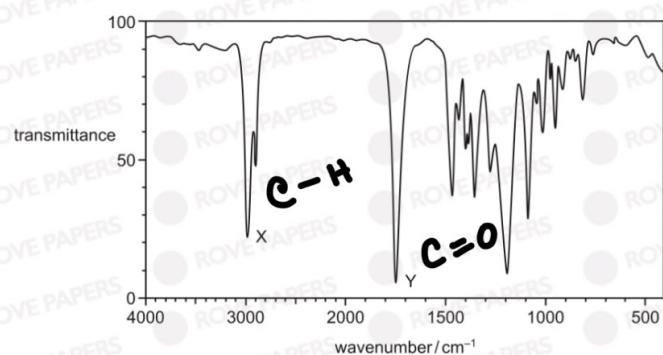


Peaks are always the minimum points

Misc. Notes

Mass Spectrometry

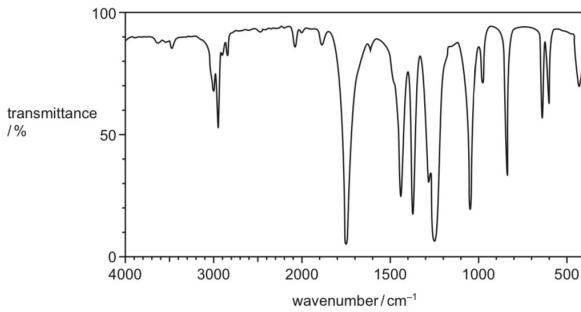
The infra-red spectrum of a substance with empirical formula C_2H_4O is shown.



During molecular fragmentation, 1 fragment becomes positively charged and the other becomes a free radical. **THIS IS ALWAYS THE CASE.** However which fragment becomes positively charged and which one becomes a free radical is not fixed.



30 The infra-red spectrum shown was obtained from compound G.

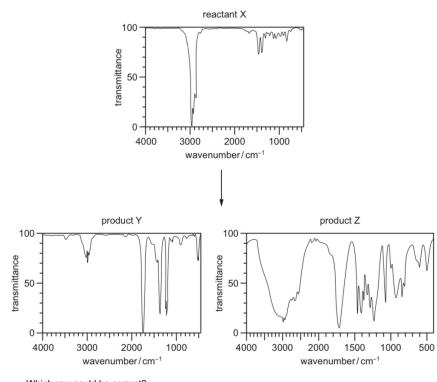


What could be compound G?

- A CH_3COCH_2OH
- B $CH_3CH_2CO_2H$
- C $CH_3CO_2CH_3$
- D $CH_3CHCHCH_3$

Carboxylic acid peaks come down more

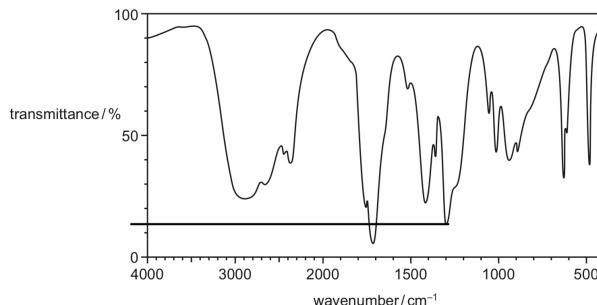
30 When reactant X is treated with a suitable reagent, products Y and Z are formed. Infrared spectra of X, Y and Z are shown.



Which row could be correct?

	X	Y	Z
A	2,3-dimethylpent-2-ene	propane	butanone
<input checked="" type="checkbox"/> B	2-methylpent-2-ene	propane	propanoic acid
C	pent-2-ene	ethanoic acid	propanoic acid
D	propyl propanoate	propan-1-ol	propanoic acid

29 Compound X has the infra-red spectrum shown.



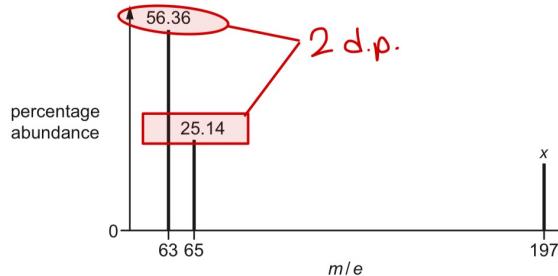
What could be the identity of compound X?

- A ethanoic acid
- B ethanol
- C ethylethanoate
- D propanone

show an absorption at 2500-3000 (cm⁻¹) because of RCO₂-H / O-H in RCO₂H / carboxyl(ic acid)

CANNOT write ONLY OH,
MUST specify to which
functional group the -OH
belongs to

(d) Tumbaga is an alloy of copper and gold. A sample of tumbaga was analysed. The mass spectrum of the sample is shown.



(i) Calculate the percentage abundance of gold, x, in the sample of tumbaga.

$$\% \text{ abundance} = (100 - 56.36 - 25.14) \\ = 18.5\%$$

$$x = 18.5 \dots \dots \dots \% [1]$$

(ii) Calculate the relative atomic mass, A_r , of the copper present in this sample. Give your answer to two decimal places.

$$\frac{56.36 \times 63}{56.36 + 25.14} + \frac{25.14 \times 65}{56.36 + 25.14}$$

$$43.57 + 20.05$$

- 1

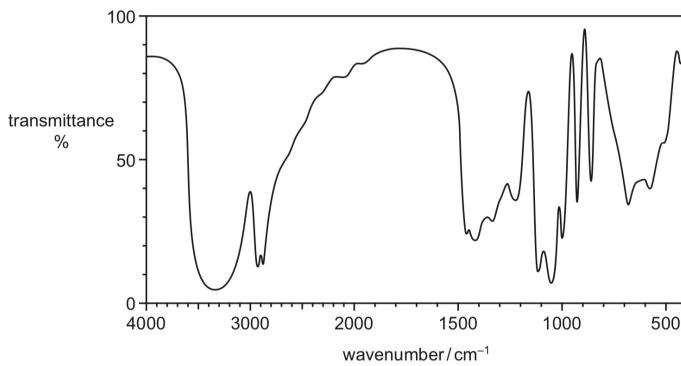
$$= 63.6$$

$$A_r (\text{Cu}) = 63.62 \dots \dots \dots [2]$$

[Total: 11]

Answer must be correct to 2 d.p.
following the pattern of the question

30 The infra-red spectrum of compound L is shown.



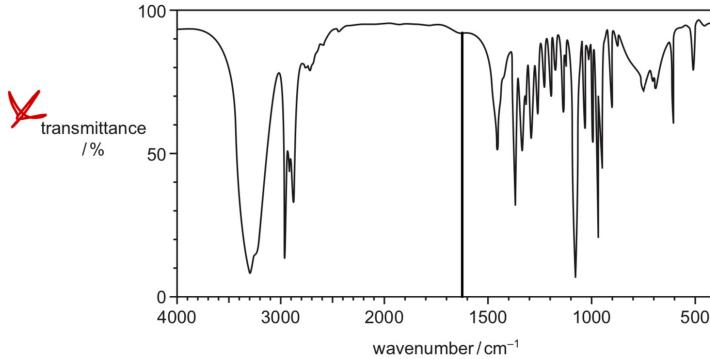
What could be the structure of L?

- A HOCH₂COCH₂OH
- B HOCH₂CH(OH)CHO
- C HOCH₂CH(OH)CH₂OH
- D HOCH₂CH₂COOH

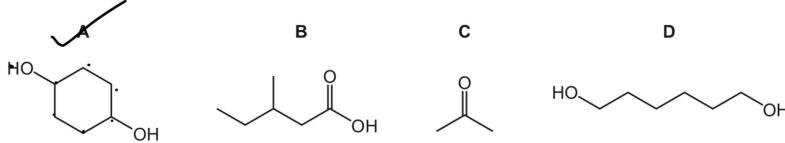
30 Substance T was analysed and found to contain 62.07% carbon, 10.34% hydrogen and 27.59% oxygen.

The infra-red spectrum of substance T is shown.

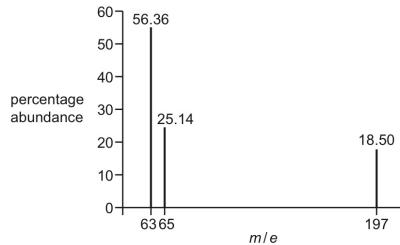
w19-12



Which substance could be T?



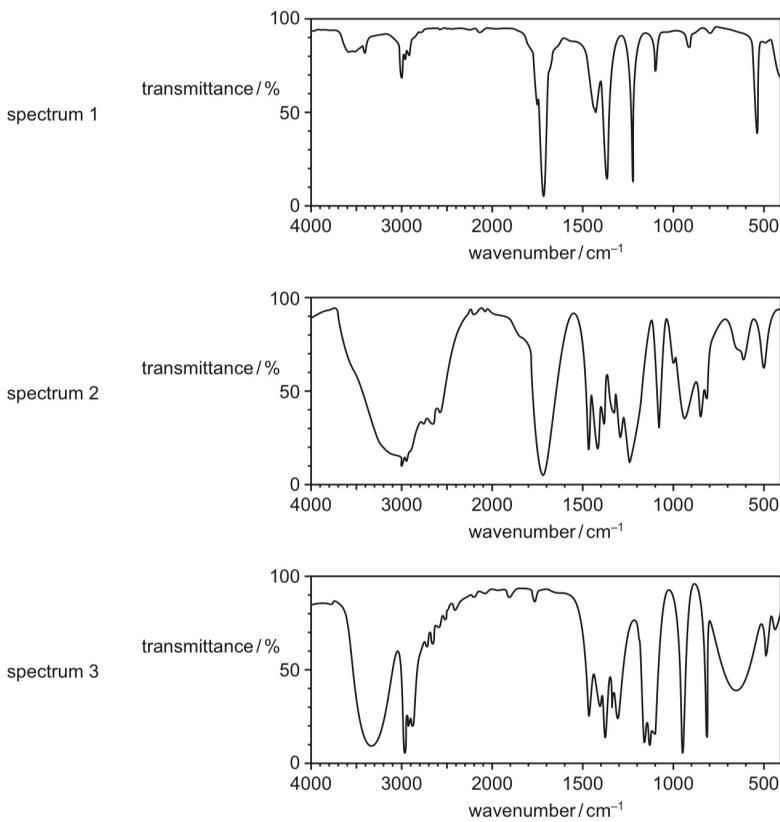
2 The mass spectrum of an alloy of copper and gold is shown.



Which expression can be used to calculate the relative atomic mass, A_r , of copper present in this sample?

- A $\frac{(56.36 \times 63) + (25.14 \times 65)}{(56.36 + 25.14 + 18.50)}$
- B $\frac{(56.36 \times 63) + (25.14 \times 65) + (18.50 \times 197)}{(56.36 + 25.14 + 18.50)}$
- C $\frac{(56.36 \times 63) + (25.14 \times 65)}{(56.36 + 25.14)}$
- D $\frac{(56.36 \times 63) + (25.14 \times 65)}{(63 + 65)}$

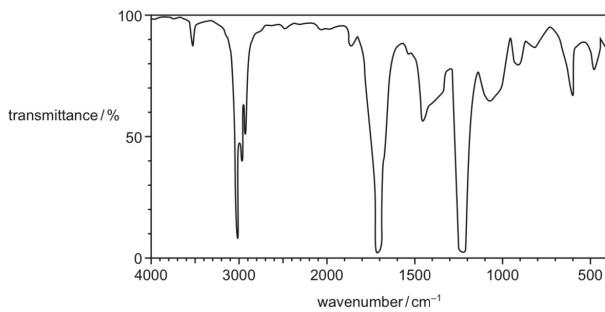
30 The infra-red spectra of three organic compounds are shown.



What could the three compounds be?

	spectrum 1	spectrum 2	spectrum 3
A	propanoic acid	propanone	propan-2-ol
B	propanone	propanoic acid	propan-2-ol
C	propanone	propan-2-ol	propanoic acid
D	propan-2-ol	propanoic acid	propanone

40 The infrared spectrum of a compound is shown.



bond	functional groups containing the bond	characteristic infrared absorption range (in wavenumbers) cm^{-1}
C–O	hydroxy, ester	1040–1300
C=C	aromatic compound, alkene	1500–1680
C=O	amide carbonyl, carboxyl ester	1640–1690 1670–1740 1710–1750
C≡N	nitrile	2200–2250
C–H	alkane	2850–2950
N–H	amine, amide	3300–3500
O–H	carboxyl hydroxy	2500–3000 3200–3600

Which functional group could the compound contain?

- A alcohol
- B carboxylic acid
- C ester
- D nitrile