

Solving structures with mass, IR and NMR spectra

Chemistry grades 11-12 (A Level · IB · Class 11-12) · Worksheet

Name: _____ Date: _____ Class: _____

These 20 problems train you to read mass, infrared and NMR data. They start with single facts, such as the molecular ion or one absorption, and move to combined structure determination at A Level and IB standard.

Write your reasoning clearly. Examiners reward each piece of evidence, so state the signal, what it shows and the group it indicates.

Level: Chemistry grades 11-12 (A Level · IB · Class 11-12) · **Curriculum:** IB S3.2

Problem 1 Molecular ion of ethanol (easy)

Aarav in Pune runs a sample of ethanol, $\text{C}_2\text{H}_6\text{O}$. The mass spectrum has M^+ at m/z 46 and a strong fragment at m/z 31.

1. State what the molecular ion tells you.
2. Show that m/z 46 fits $\text{C}_2\text{H}_6\text{O}$ ($\text{C} = 12$, $\text{H} = 1$, $\text{O} = 16$).
3. Calculate the m/z of CH_2OH^+ and say whether it explains the peak at 31.

Problem 2 Matching IR bands (easy)

Wanjiru in Nairobi records four absorptions: 3350 cm^{-1} (broad), 1715 cm^{-1} (strong), 2240 cm^{-1} and 1650 cm^{-1} .

1. Match each to one of these bonds: $\text{C}\equiv\text{N}$, $\text{C}=\text{C}$, $\text{C}=\text{O}$ and $\text{O}-\text{H}$ in an alcohol.
2. State which absorption is in the fingerprint region, if any.

Problem 3 Counting hydrogen environments (easy)

Emma in Leeds studies proton NMR.

1. State the number of signals for $\text{CH}_3\text{CH}_2\text{CH}_3$, CH_3OCH_3 , $\text{CH}_3\text{CH}_2\text{OH}$ and benzene.
2. Explain why CH_3OCH_3 gives only one signal.

Problem 4 Predicting the splitting (easy)

Chiamaka in Lagos predicts the proton NMR of 1,1-dichloroethane, CH_3CHCl_2 , and 1,2-dichloroethane, $\text{ClCH}_2\text{CH}_2\text{Cl}$.

1. State the splitting and integration of each signal in the first compound.
2. State the splitting of the signal in the second compound and explain.

Problem 5 Wavelength to wavenumber (easy)

An IR beam has wavelength 5.88 μm and another has wavelength 3.00 μm . Use 1 μm = 10^{-4} cm.

1. Calculate the wavenumber of each in cm^{-1} .
2. Say which bond each is likely to excite, from C=O and O-H.

Problem 6 Counting carbons from M+1 (medium)

Diego in Texas analyses an ester. The M^+ peak at m/z 88 has a height of 55.0 mm and the $\text{M}+1$ peak has a height of 2.4 mm. Each carbon contributes 1.1 % of the M^+ height.

1. Calculate the number of carbon atoms.
2. The ester contains two oxygen atoms. Work out its molecular formula.

Problem 7 Two ketone isomers (medium)

A ketone of M^+ at m/z 86 has fragment peaks at 57 and 29, and no peak at 43. Candidates are pentan-2-one and pentan-3-one.

1. Calculate the m/z of $\text{CH}_3\text{CH}_2\text{CO}^+$ and of C_2H_5^+ .
2. Identify the ketone.
3. State the two fragment peaks the other ketone would give instead.

Problem 8 Alcohol or ketone (medium)

Two isomers have formula $\text{C}_3\text{H}_6\text{O}$: propanone and prop-2-en-1-ol, $\text{CH}_2=\text{CHCH}_2\text{OH}$. A spectrum shows a strong absorption at 1715 cm^{-1} and no absorption between 3200 and 3550 cm^{-1} .

1. Identify the compound.
2. State two absorptions the other compound would show.

Problem 9 ^{13}C environments (medium)

Predict the number of ^{13}C NMR signals for each compound.

1. Pentane.
2. Propanone.
3. 2-methylpropane.
4. Ethyl ethanoate.
5. 1,4-dimethylbenzene.

Problem 10 Propanoic acid data (medium)

A compound has M^+ at m/z 74 and formula $\text{C}_3\text{H}_6\text{O}_2$. IR shows a very broad absorption from 2500 to 3300 cm^{-1} and a strong absorption at 1710 cm^{-1} . Proton NMR shows δ 11.5 (singlet, 1H), δ 2.38 (quartet, 2H) and δ 1.16 (triplet, 3H).

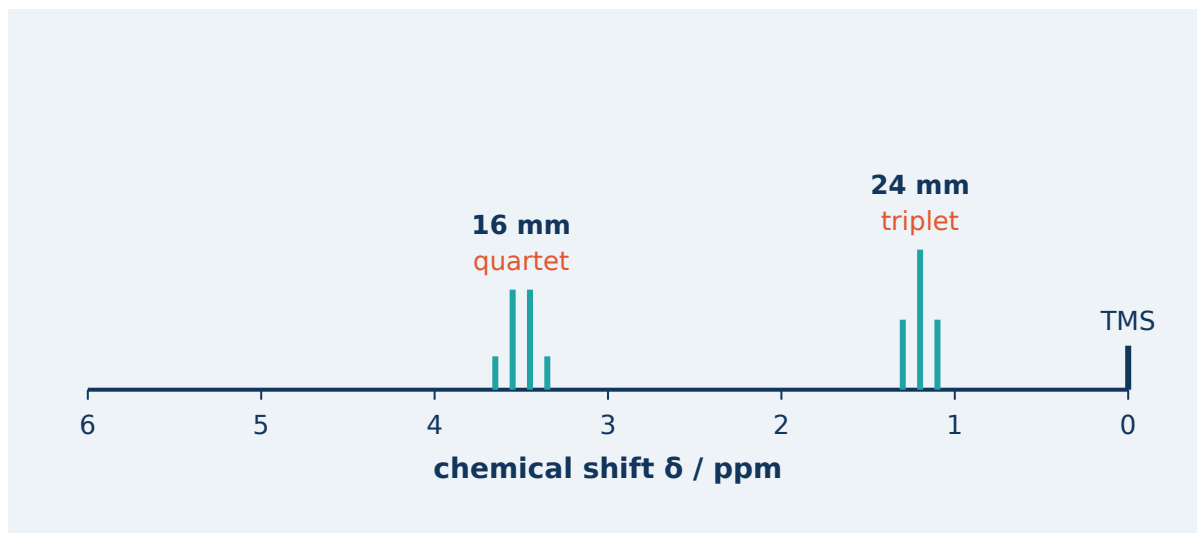
1. Identify the functional group.
2. Assign each NMR signal.

3. Give the structure and name.

Problem 11 Reading integration traces (medium)

The NMR trace in the diagram has formula $C_4H_{10}O$ and no IR absorption above 3000 cm^{-1} . The integral heights are 24 mm and 16 mm.

1. Calculate the ratio of hydrogens.
2. Calculate the number of hydrogens in each signal.
3. Identify the compound.



Proton NMR of an unknown with formula $C_4H_{10}O$ and integral heights.

Problem 12 Why TMS is the reference (medium)

1. State the formula of TMS.
2. Give two reasons for using TMS as the reference in proton NMR.
3. Explain why the solvent for NMR is often deuterated chloroform, $CDCl_3$.

Problem 13 Halogen isotope patterns (medium)

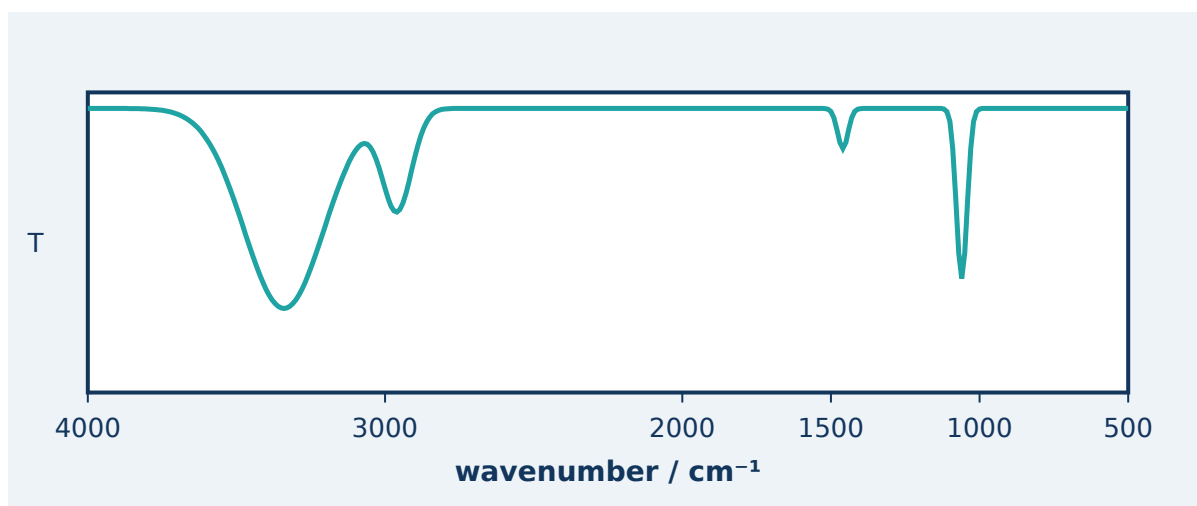
Chlorine is 75 % ^{35}Cl and 25 % ^{37}Cl . Bromine is about 50 % ^{79}Br and 50 % ^{81}Br .

1. Predict the m/z values and relative heights of the molecular ion peaks of 1-chloropropane, C_3H_7Cl .
2. Predict the same for 1-bromobutane, C_4H_9Br .

Problem 14 An alcohol from its IR (medium)

Use the infrared spectrum of a compound of formula $C_4H_{10}O$.

1. Identify the bond responsible for the broad absorption near 3340 cm^{-1} .
2. Explain why the spectrum shows that the compound is not ethoxyethane.
3. Explain why the strong absorption near 1060 cm^{-1} is not used for a firm identification.

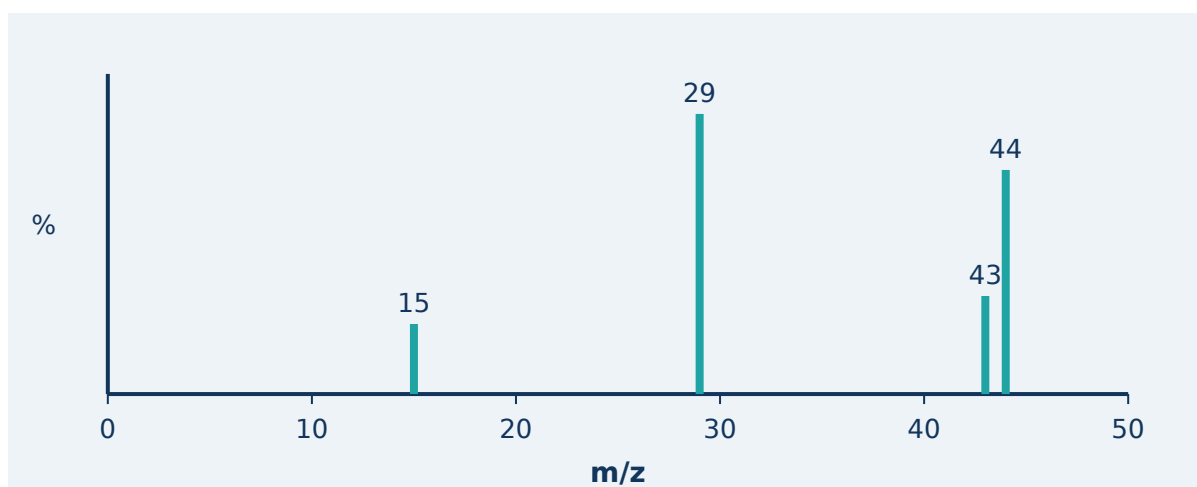


Infrared spectrum of a compound with formula $C_4H_{10}O$.

Problem 15 Fragments of a small aldehyde (medium)

The mass spectrum in the diagram is for a compound of formula C_2H_4O with an IR absorption at 1730 cm^{-1} .

1. State the m/z of the molecular ion.
2. Assign the peaks at 15, 29 and 43.
3. Identify the compound.



Mass spectrum of an unknown with formula C_2H_4O .

Problem 16 A full ester analysis (hard)

A compound has M^+ at m/z 102 and formula $C_5H_{10}O_2$. IR: strong absorption at 1738 cm^{-1} and none above 3000 cm^{-1} . Proton NMR: δ 1.12 (triplet, 3H), δ 1.25 (triplet, 3H), δ 2.31 (quartet, 2H), δ 4.12 (quartet, 2H). ^{13}C NMR shows 5 signals, including one at 174 ppm. MS peaks at 57 and 29.

1. State the functional group.
2. Assign the four proton signals with reasons.
3. Name the compound and explain how the ^{13}C data support it.

Problem 17 A nitrogen compound (hard)

A compound has M^+ at m/z 55 and contains C, H and N only. IR shows a sharp absorption at 2250 cm^{-1} and no absorption near 1700 or 3300 cm^{-1} . Proton NMR: δ 1.3 (triplet, 3H) and δ 2.4 (quartet, 2H). ^{13}C NMR has 3 signals, one near 120 ppm .

1. Work out the molecular formula.
2. Identify the group giving the IR absorption.
3. Deduce and name the structure.

Problem 18 A bromoalkane with a single carbon branch (hard)

A compound has M^+ peaks at m/z 150 and 152 of equal height. The $M+1$ peak is 5.5 % of the height of M^+ . Proton NMR: δ 1.05 (singlet, 9H) and δ 3.3 (singlet, 2H). ^{13}C NMR has 3 signals.

1. Calculate the number of carbon atoms.
2. Work out the molecular formula ($\text{C} = 12$, $\text{H} = 1$, $\text{Br} = 79$).
3. Deduce the structure and explain why both signals are singlets.

Problem 19 Telling aldehyde isomers apart (hard)

Butanal, butanone and 2-methylpropanal all have formula $\text{C}_4\text{H}_8\text{O}$. An unknown shows 3 signals in its ^{13}C spectrum. Its proton NMR has δ 9.6 (doublet, 1H), δ 2.4 (multiplet, 1H) and δ 1.1 (doublet, 6H).

1. Predict the number of ^{13}C signals for each of the three isomers.
2. Identify the unknown.
3. Explain why the signal at δ 9.6 is a doublet.

Problem 20 Propanol isomers in forensics (hard)

Kofi in Accra compares two samples of $\text{C}_3\text{H}_8\text{O}$. Sample P has base peak at m/z 31 and sample Q has base peak at m/z 45. Both have M^+ at m/z 60.

1. Calculate the m/z of CH_2OH^+ and of CH_3CHOH^+ .
2. Identify P and Q.
3. Explain why their IR spectra above 1500 cm^{-1} look alike and how ^{13}C NMR separates them.