

Solving structures with mass, IR and NMR spectra

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

Name: _____ Date: _____ Class: _____ Mark: ____ / 20

This test covers mass spectra, infrared absorption, proton and carbon-13 NMR. Use the reference ranges in the lesson. Show all working for calculations, and write short, specific explanations.

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

Time: 45 minutes · 8 questions · Total: 20 marks · Calculator allowed

Question 1 Reading a carbonyl band (2 marks)

An IR spectrum has a strong absorption at 1735 cm^{-1} , an absorption at 2960 cm^{-1} and nothing between 2500 and 3600 cm^{-1} .

- Identify the bond responsible for 1735 cm^{-1} . (1 mark)
- Explain why the compound is not a carboxylic acid. (1 mark)

Question 2 Halogen molecular ions (3 marks)

The mass spectrum of 2-bromopropane, $\text{CH}_3\text{CHBrCH}_3$, has two molecular ion peaks.

- Calculate their m/z values ($\text{C} = 12$, $\text{H} = 1$, ^{79}Br and ^{81}Br). (2 marks)
- State the ratio of their heights and the reason. (1 mark)

Question 3 Tertiary alcohol NMR (3 marks)

2-methylpropan-2-ol is $(\text{CH}_3)_3\text{COH}$.

- State the number of signals in its proton NMR spectrum and their integration ratio. (2 marks)
- Explain why both signals are singlets. (1 mark)

Question 4 Hexane isomers in ^{13}C NMR (3 marks)

State the number of signals in the ^{13}C NMR spectrum of each isomer of C_6H_{14} .

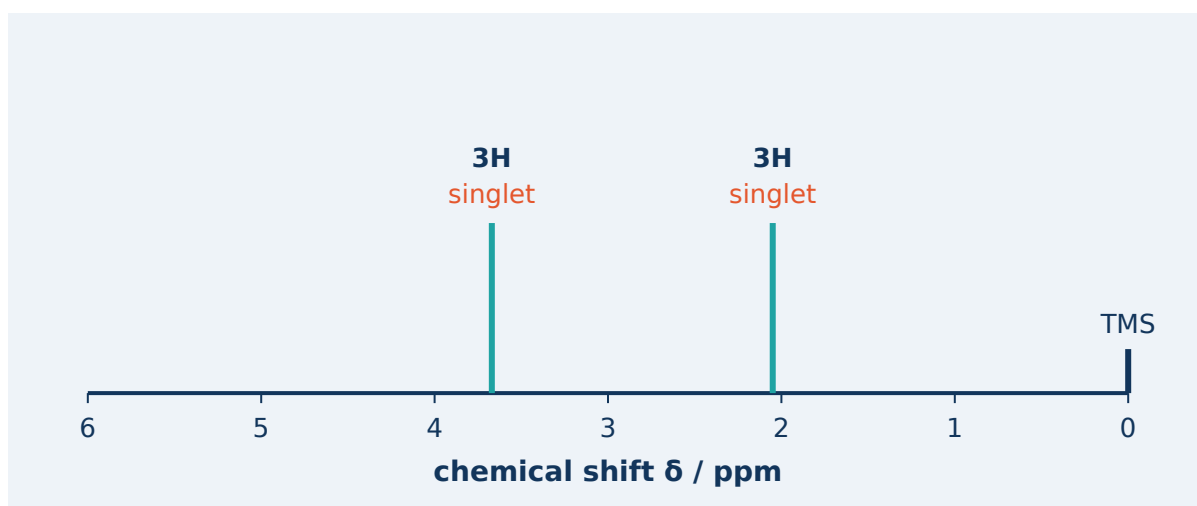
- Hexane. (1 mark)

- b. 2,2-dimethylbutane. (1 mark)
- c. 2,3-dimethylbutane. (1 mark)

Question 5 Identify a small ester (3 marks)

A compound has M^+ at m/z 74, formula $C_3H_6O_2$, and an IR absorption at 1745 cm^{-1} . Its proton NMR is shown.

- a. Explain why there are two singlets of equal height. (2 marks)
- b. Name the compound. (1 mark)



Proton NMR of a compound with $M_r = 74$.

Question 6 Wavenumber and bond strength (2 marks)

A $C=O$ bond absorbs at 1715 cm^{-1} .

- a. Calculate the wavelength in μm ($1\text{ }\mu\text{m} = 10^{-4}\text{ cm}$). (1 mark)
- b. Explain why $C=O$ absorbs at higher wavenumber than $C=C$. (1 mark)

Question 7 Deuterium oxide shake (2 marks)

A few drops of D_2O are shaken with ethanol and the proton NMR is run again. Predict what happens to the O-H signal and explain. (2 marks)

Question 8 Counting carbons (2 marks)

In a mass spectrum, M^+ has height 40.0 mm and the $M+1$ peak has height 3.08 mm. Each carbon contributes 1.1 %. Calculate the number of carbon atoms. (2 marks)