

Solving structures with mass, IR and NMR spectra

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

Model answers and marking points follow. Give credit for each correct step, allow error carried forward in a later part, and do not award marks for a correct answer with a contradicting reason.

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

Question 1 Reading a carbonyl band (2 marks)

- a. **C=O**.
- b. A carboxylic acid has a very broad O-H absorption from 2500 to 3300 cm^{-1} , which is absent.

Marking: 1 for C=O; 1 for absence of O-H.

Question 2 Halogen molecular ions (3 marks)

- a. $\text{C}_3\text{H}_7^{79}\text{Br}$: $36 + 7 + 79 = \mathbf{122}$; $\text{C}_3\text{H}_7^{81}\text{Br}$: $36 + 7 + 81 = \mathbf{124}$.
- b. **1 : 1**, because the two bromine isotopes are almost equally abundant.

Marking: 1 for each m/z ; 1 for ratio with reason.

Question 3 Tertiary alcohol NMR (3 marks)

- a. **2 signals**, ratio **9 : 1** (three equivalent CH_3 and one OH).
- b. The CH_3 hydrogens have no hydrogens on adjacent carbons, and the OH hydrogen does not split, so neither is split.

Marking: 1 for two signals; 1 for 9 : 1; 1 for reason.

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

- a. Hexane: **3**.
- b. 2,2-dimethylbutane: **4** (three equivalent CH_3 , quaternary C, CH_2 , CH_3).
- c. 2,3-dimethylbutane: **2** (four equivalent CH_3 and two equivalent CH).

Marking: 1 mark each.

Question 5 Identify a small ester (3 marks)

a. The compound has two CH₃ groups, one next to C=O and one next to oxygen, and neither has hydrogens on adjacent atoms, so each is a singlet; each has 3 H, so the heights are equal.

b. **Methyl ethanoate**, CH₃COOCH₃.

Marking: 1 for no adjacent hydrogens; 1 for 3H : 3H; 1 for methyl ethanoate.

Question 6 Wavenumber and bond strength (2 marks)

a. $1 \div 1715 = 5.83 \times 10^{-4} \text{ cm} = \mathbf{5.83 \mu m}$.

b. The C=O bond is stronger than the C=C bond, so it vibrates at higher frequency.

Marking: 1 for 5.83 μm; 1 for stronger bond.

Question 7 Deuterium oxide shake (2 marks)

The O-H signal **disappears**. The O-H hydrogen exchanges with deuterium to give O-D, and deuterium does not absorb in proton NMR.

Marking: 1 for disappears; 1 for exchange with deuterium.

Question 8 Counting carbons (2 marks)

$3.08 \div 40.0 = 7.7 \%$; $7.7 \div 1.1 = 7.0$, so **7 carbon atoms**.

Marking: 1 for 7.7 %; 1 for 7.