NMR spectroscopy

AQA 7405 · A level

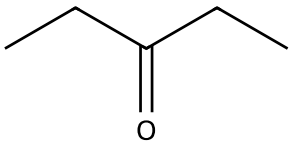
Show your working where needed. Check the worked answers when you finish.

Name _____ Date _____

1. Count carbon environments

How many signals does A give in proton-decoupled ^{13}C NMR? Explain your count.

A



2. Use integration and symmetry

Predict the number of signals for propanone, CH_3COCH_3, in ^{1}H NMR. Give the integration as a proton count and explain the splitting.

3. Predict the integration and splitting

For ethanol, predict the splitting pattern of each carbon-bound proton group and the ratio of the peak areas. Ignore coupling to the exchangeable OH proton.

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4. Choose a reference

Why does TMS give one ^{1}H NMR reference signal, and what is its δ value? State one reason for using a deuterated solvent.

5. Identify an unknown

Use your board's data sheet for NMR shifts and infrared bands in this set.

A compound with molecular formula $C_3H_6O_2$ gives two ^{1}H NMR singlets at δ 2.1 and 3.7, each representing 3H. Suggest a structure and assign both signals.

6. Use two carbon shifts

Compound P gives a ^{13}C signal at δ 172. Compound Q gives one at δ 208. Both have C=O. Suggest one different carbonyl class consistent with each shift and explain why a carbonyl peak alone does not identify P uniquely.

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7. Combine IR and NMR

An unknown $C_3H_6O_2$ compound has a broad IR absorption at 2500-3000 cm^{-1} and a strong band at 1715 cm^{-1}. Its ^1H NMR includes a 3H triplet and a 2H quartet.

Deduce its structure and show how the evidence supports it.

8. Solve a four-signal spectrum

An ester $C_5H_{10}O_2$ gives the following ^1H NMR signals. δ 1.1 (triplet, 3H), δ 1.3 (triplet, 3H), δ 2.3 (quartet, 2H) and δ 4.1 (quartet, 2H).

Deduce its structure and identify the two CH_2 environments.

9. Extra challenge · Distinguish two esters

An ester $C_5H_{10}O_2$ gives four ^{13}C signals, including δ 171. Its ^1H signals are a 6H doublet at δ 1.2, a 3H singlet at δ 2.1 and one complex 1H signal at δ 4.9. Treat δ 4.9 as a proton on carbon directly bonded to an ester oxygen.

Use both spectra to deduce the ester and explain why ethyl propanoate fails. Give the products of hydrolysis with hot aqueous NaOH.

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Worked answers

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1. Count carbon environments

Three. The two CH_3 carbons are equivalent and the two CH_2 carbons are equivalent. The central carbonyl carbon gives a third signal.

2. Use integration and symmetry

One signal represents six protons because the two methyl groups are equivalent. The adjacent carbonyl carbon has no hydrogen atoms, so the signal is a singlet.

3. Predict the integration and splitting

CH_3 gives a triplet because two adjacent CH_2 protons split it. CH_2 gives a quartet because three adjacent CH_3 protons split it. The triplet-to-quartet area ratio is 3:2.

4. Choose a reference

TMS defines δ = 0 ppm. Its four methyl groups are equivalent, so its twelve protons contribute to a single reference signal.

A deuterated solvent minimises the solvent signal in a ^1H spectrum because deuterium is detected at a different frequency.

5. Identify an unknown

$CH_3C(=O)OCH_3$, methyl ethanoate. The δ 2.1 signal is from CH_3 directly bonded to the carbonyl carbon. The δ 3.7 signal is from OCH_3.

Neither methyl group has adjacent carbon-bound protons to split its signal in the usual simple model.

6. Use two carbon shifts

The δ 172 signal is consistent with an ester or a carboxylic acid carbonyl. The δ 208 signal is consistent with a ketone or aldehyde carbonyl. P could be either an acid or an ester, so use evidence such as an IR O-H band or proton NMR to decide.

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Worked answers

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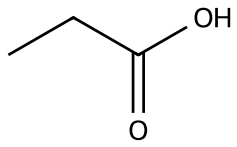
7. Combine IR and NMR

The wide O-H band and the C=O band together support a carboxylic acid. A 3H triplet and a 2H quartet fit an ethyl group.

The CH_2 is next to three H atoms on CH_3, and CH_3 is next to two on CH_2. The structure is CH_3CH_2COOH, propanoic acid.

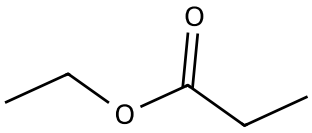


Propanoic acid

8. Solve a four-signal spectrum

Ethyl propanoate, $CH_3CH_2C(=O)OCH_2CH_3$. Two quartet-triplet pairs are consistent with two distinct ethyl fragments.

The CH_2 bonded to O gives the δ 4.1 quartet. The CH_2 next to the carbonyl on the other side of the ester gives the δ 2.3 quartet.



Ethyl propanoate

9. Extra challenge · Distinguish two esters

The 6H doublet implies two equivalent methyl groups adjacent to one CH proton. The δ 4.9 proton is on the carbon bonded to the ester oxygen. The δ 2.1 singlet is CH_3 attached to the carbonyl, so the compound is $CH_3COOCH(CH_3)_2$.

It gives four carbon environments because both terminal methyl carbons of the isopropyl group are equivalent. Ethyl propanoate has five distinct environments and two separate ethyl groups. Hydrolysis gives CH_3COONa and $(CH_3)_2CHOH$.

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