NMR spectroscopy

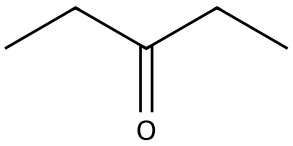
OCR A H432 · A level

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. A spectrum before and after D_2O

After shaking a sample of $HOCH_2CH_2NH_2$ with D_2O, two ^{1}H NMR signals disappear. Before shaking they represented 1H and 2H respectively. Assign the missing signals and give the area ratio of the two signals left.

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7. Combine IR and NMR

An unknown $C_3H_6O_2$ compound has a broad IR absorption at 2500-3300 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 · Use exchange and the aromatic region

A $C_8H_{10}O$ compound is ethoxybenzene, 2-phenylethanol or an ethylphenol. Its ^1H spectrum has a 3H triplet, a 2H quartet, aromatic resonances totalling 4H and a 1H signal that disappears with D_2O.

Identify the candidate and explain which evidence eliminates each alternative. Explain why the data do not identify the relative positions of substituents.

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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. A spectrum before and after D_2O

The 1H signal was from the OH proton and the 2H signal was from NH_2. These protons exchange with deuterium, which is absent from the ^1H NMR spectrum.

Both CH_2 groups retain their protons. The remaining area ratio is 2:2, or 1:1.

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Worked answers

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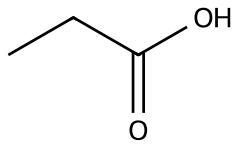
7. Combine IR and NMR

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.

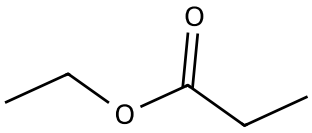


Propanoic acid

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 · Use exchange and the aromatic region

Ethylphenol fits. A 3H triplet and a 2H quartet fit an ethyl group. Four aromatic protons indicate two ring substituents. The disappearing 1H signal indicates an exchangeable OH proton.

Ethoxybenzene has no exchangeable proton and has five aromatic protons. 2-Phenylethanol has five aromatic protons and two CH_2 groups. The total aromatic integration is the same for each ethylphenol positional isomer, so further spectral evidence is needed to assign its positions.

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