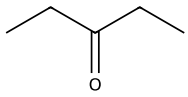
NMR spectroscopy

AQA 7405 · A level

Answer on your own paper. Show your working where needed.

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.

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.

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 ^{1}H 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 ^{1}H 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 ^{1}H 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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