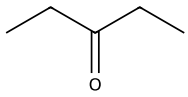
NMR spectroscopy

OCR A H432 · 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 ^1H 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 ^1H 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 ^1H 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 ^1H 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.

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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