NMR spectroscopy

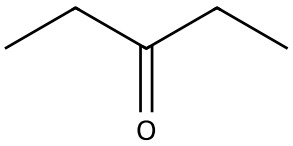
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Show your working where needed.

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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