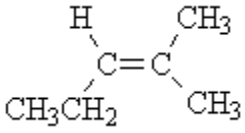
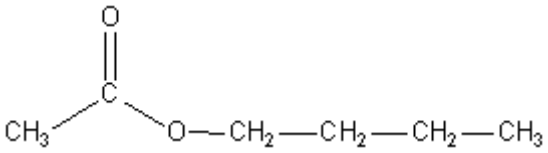
C13 NMR SPECTROSCOPY – CONCEPT TEST

QUESTION 1
How many peaks will the following compound have in its carbon NMR spectrum?



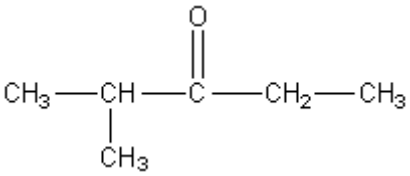
A 3
B 4
C 5
D 6

QUESTION 2
How many signals are expected in the ^{13}C NMR spectrum of butyl acetate?



A 2
B 4
C 6
D 8

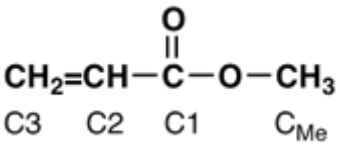
QUESTION 3
How many signals are expected in the ^{13}C NMR spectrum of ethyl isopropyl ketone?



A 1
B 3
C 5
D 7

QUESTION 4

Which of options indicates the correct order of carbon chemical shifts of the four carbons of the following compound.



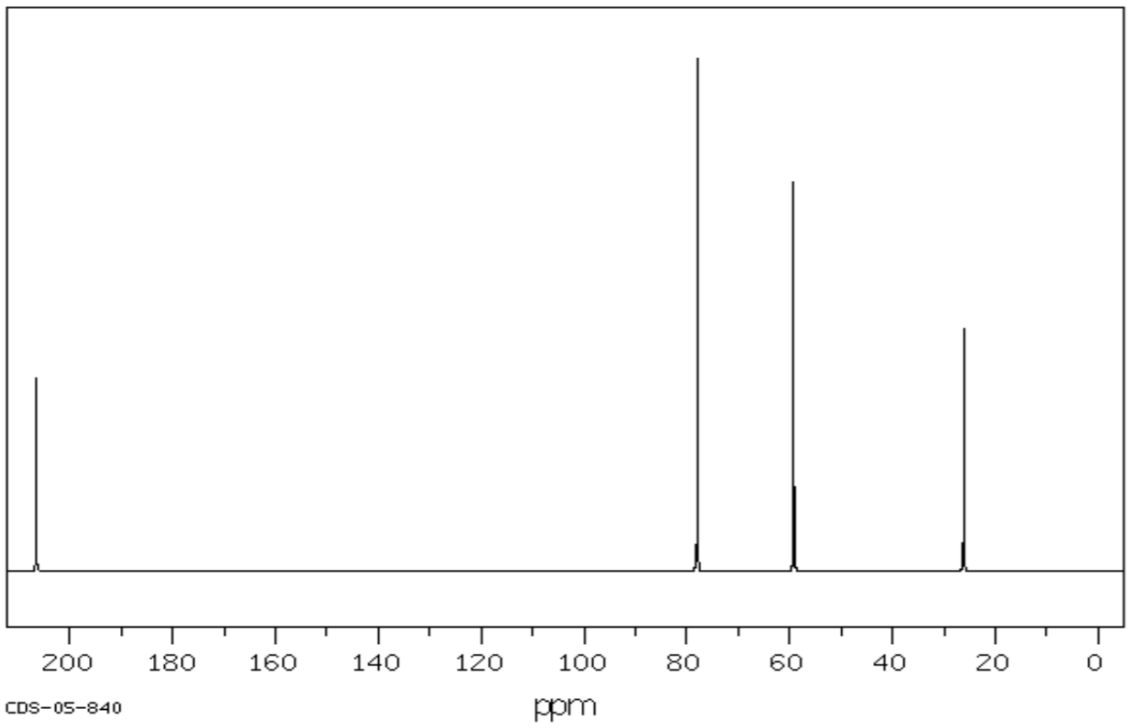
A C_{Me} < C2 < C3 < C1

B C3 < C2 < C_{Me} < C1

C C1 < C3 < C2 < C_{Me}

D C1 < C_{Me} < C2 < C3

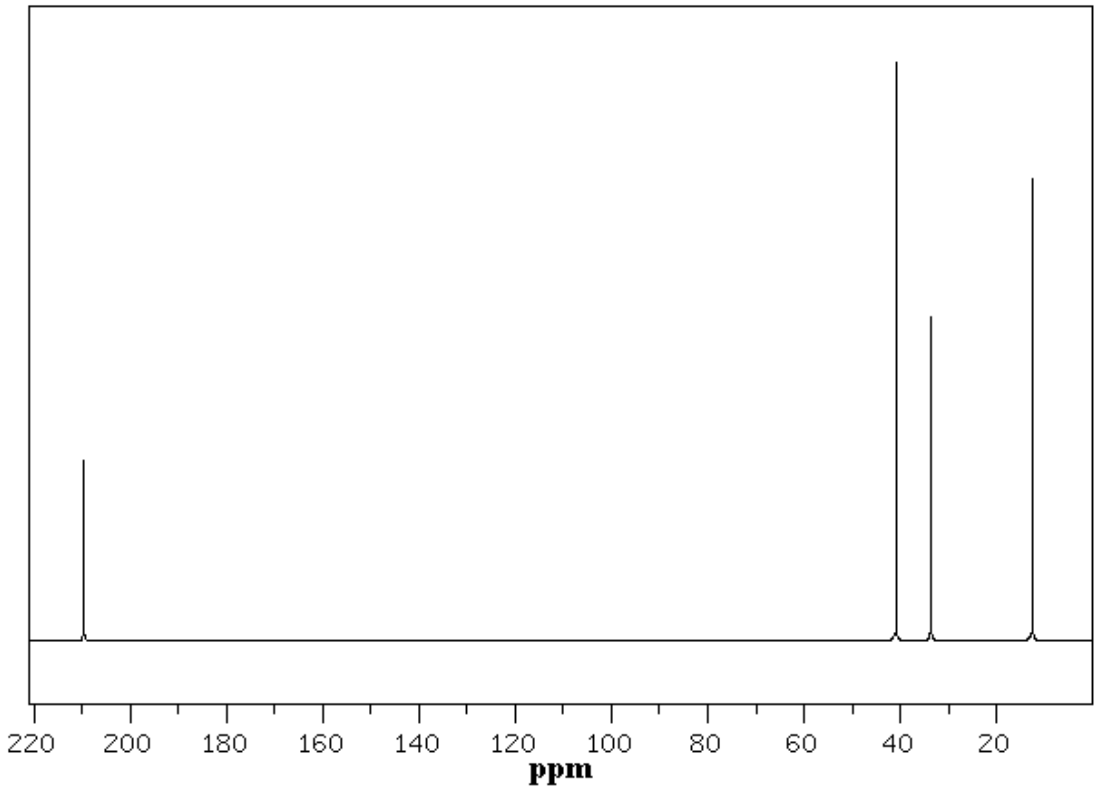
QUESTION 5
An isomer of methyl propanoate has the following C-13 NMR spectrum. Work out the probable structural formula for the compound, explaining your reasoning.



Solution

QUESTION 6

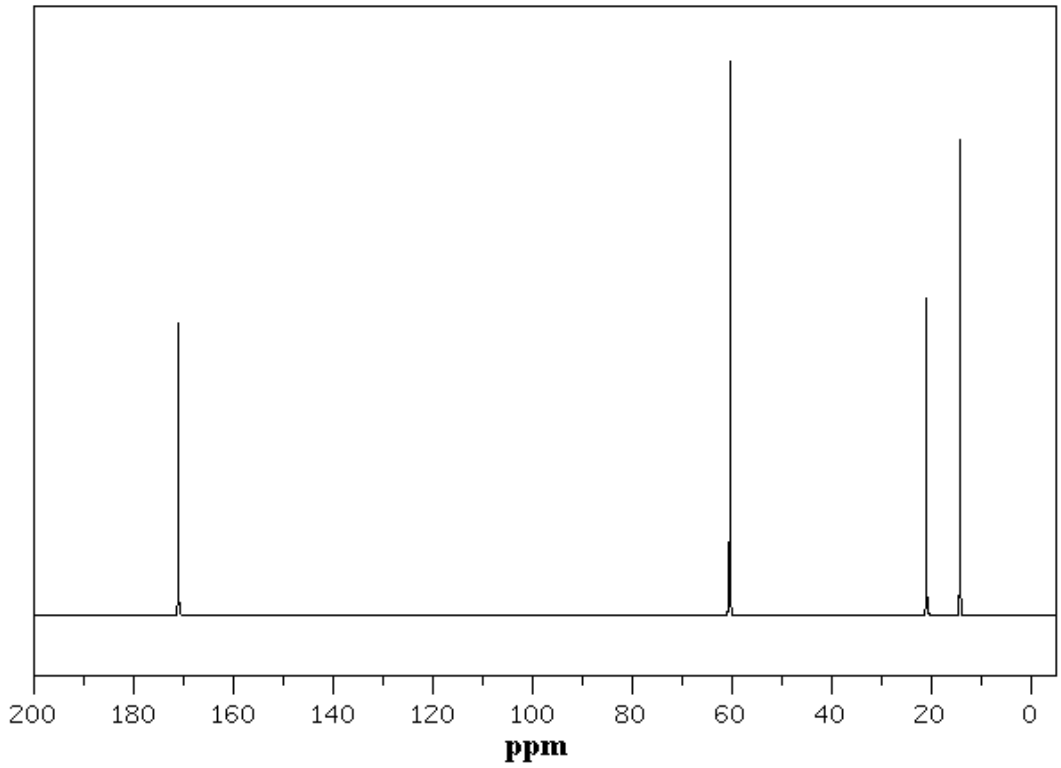
The following C13 NMR spectrum was produced by a compound with molecular formula C_4H_8O. Use this spectrum to draw a possible structure for the molecule.



Solution

QUESTION 7

The following C13 NMR spectrum was produced by a compound with molecular formula $C_4H_8O_2$. Use this spectrum to draw a possible structure for the molecule.



Solution

SOLUTIONS

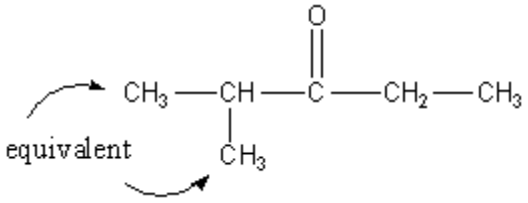
QUESTION 1 Answer is D

QUESTION 2 Answer is C

There are 6 signals for butyl acetate. Each carbon atom is chemically different, therefore, none of the carbon atoms are magnetically equivalent.

QUESTION 3 Answer is C

There are 5 peaks. Two peaks for the ethyl group; two peaks for the isopropyl group and one peak for the carbonyl carbon.



QUESTION 4 Answer is A

The chemical shift of the carbonyl carbon (C1) is the largest and those of the alkene carbons are the next largest.

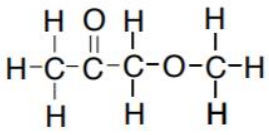
QUESTION 5

An isomer of methyl propanoate will have the molecular formula $C_4H_8O_2$. Start at the left-hand side of the spectrum.

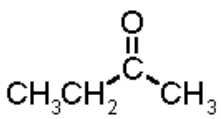
The line at 207 is likely to be a carbon in the C=O bond in a ketone. So this isn't an acid or an ester. Ketones have the C=O bond in the middle of a chain.

The lines at 59 and 78 are both due to carbons singly bonded to an oxygen, but that oxygen can't be joined to the C=O bond otherwise it would be an acid or an ester.

The line at 26 is most likely to be a CH_3 group attached to a C=O bond.

Putting that together will lead you to 

QUESTION 6



QUESTION 7