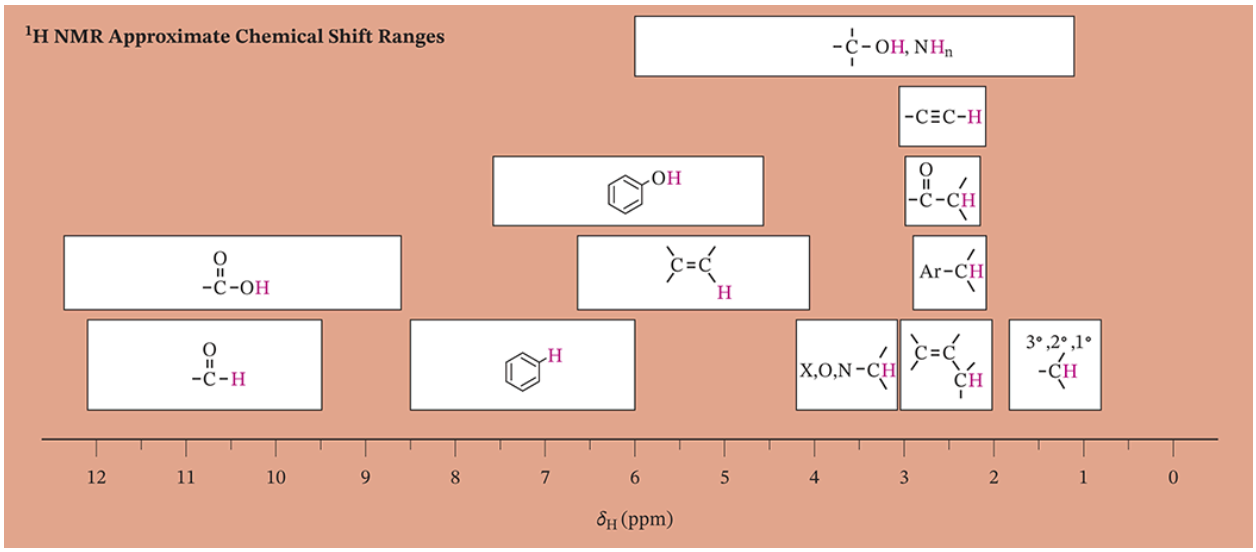
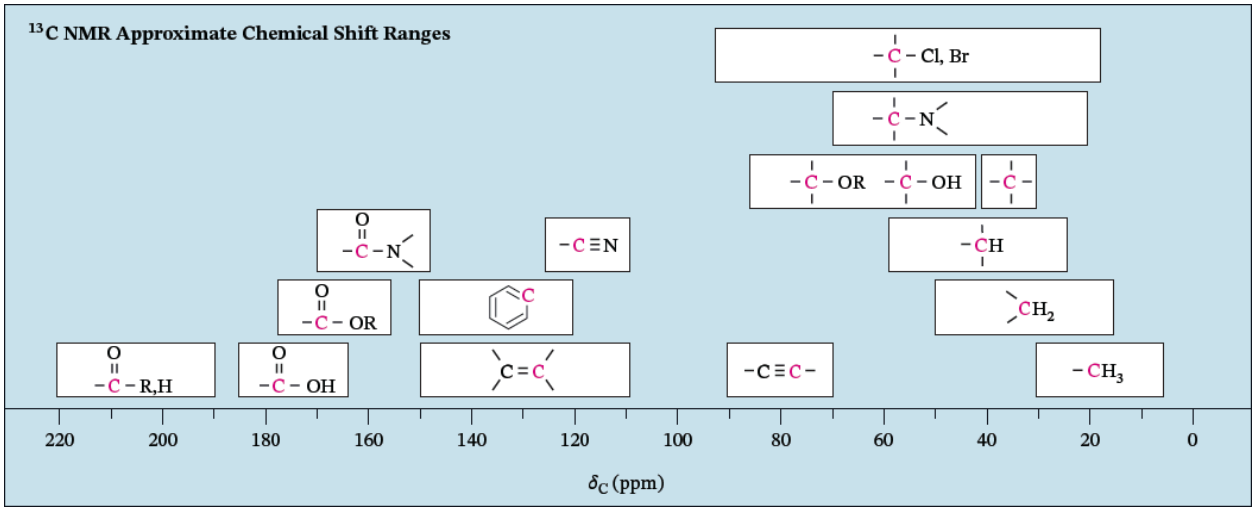
Session 17 Worksheet

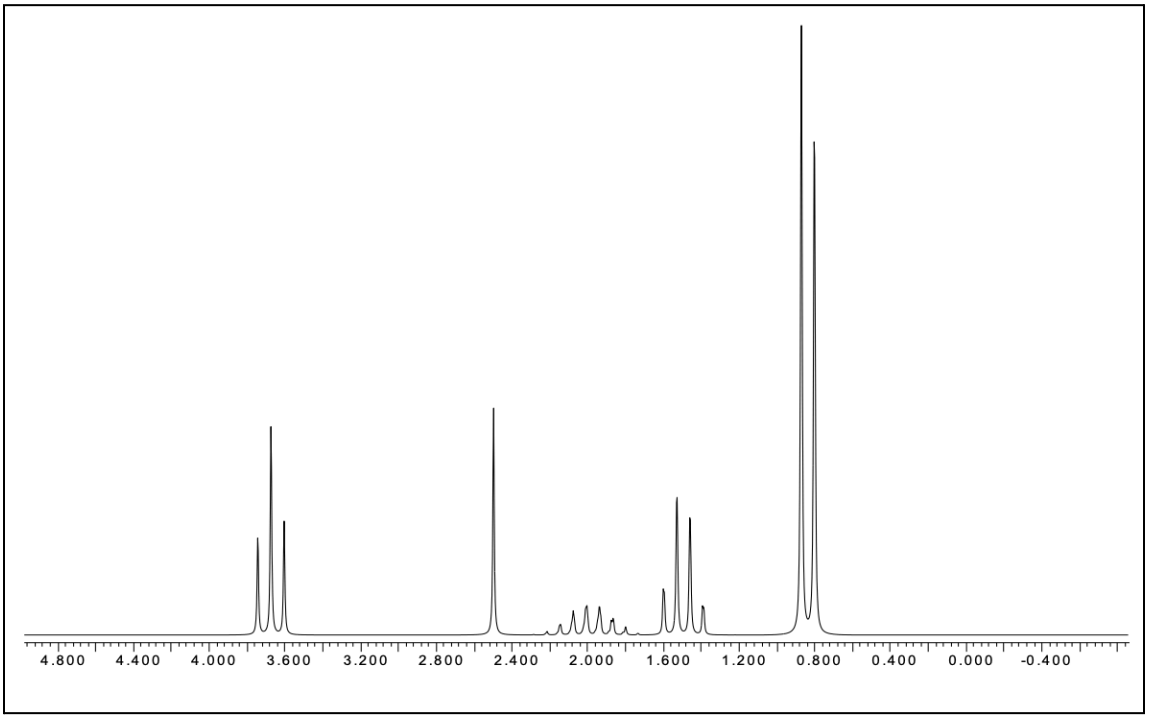
Remember these:





Continuing with ^1H NMR

Given the following molecular formula and ^1H NMR spectra, propose a structure



Given the molecular formula and signal report, propose a structure

$C_5H_{10}O$ δ = 0.95 ppm (6H, doublet)
δ = 2.10 ppm (3H, singlet)
δ = 2.43 ppm (1H, multiplet)

^{13}C NMR:

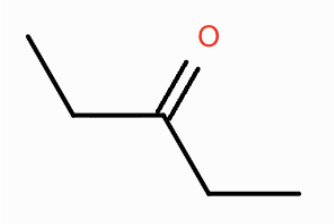
Instead of counting H environments, we're looking at _____

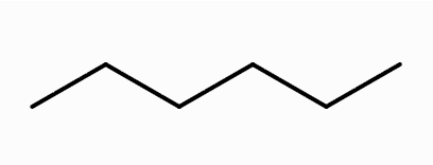
Carbon environments can also have _____

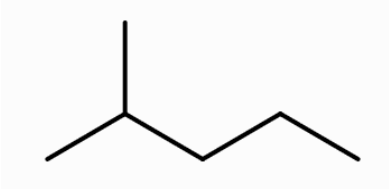
^{13}C NMR signal do not have_____, so the signals on ^{13}C NMR look like

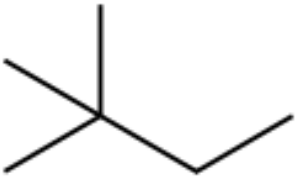
_____

Label and determine the number of carbon environments in the compounds below:



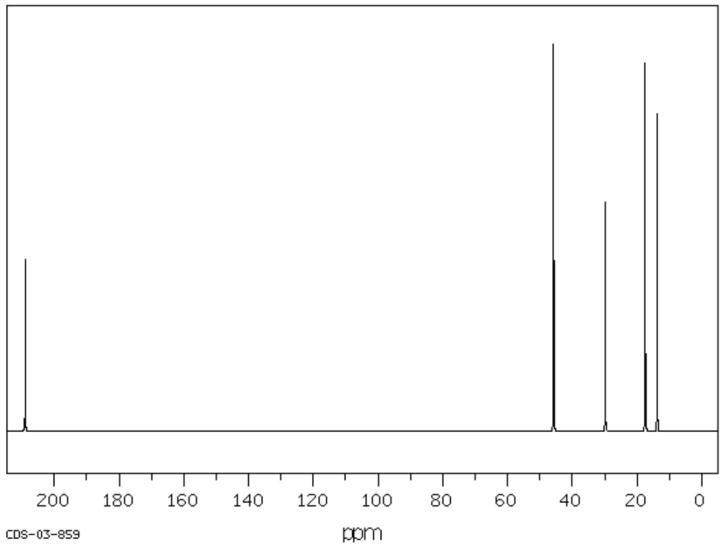




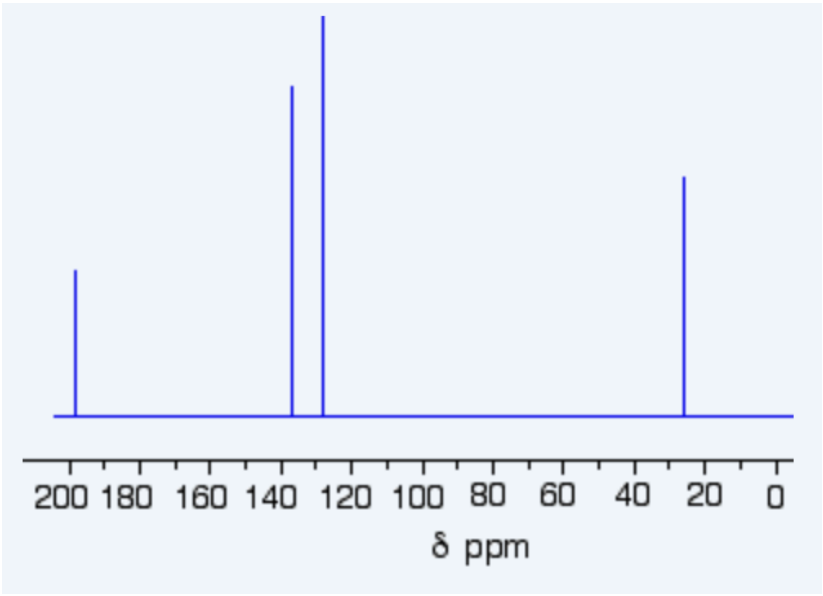


Given the molecular formula and ^{13}C NMR spectra, propose a structure for the compound

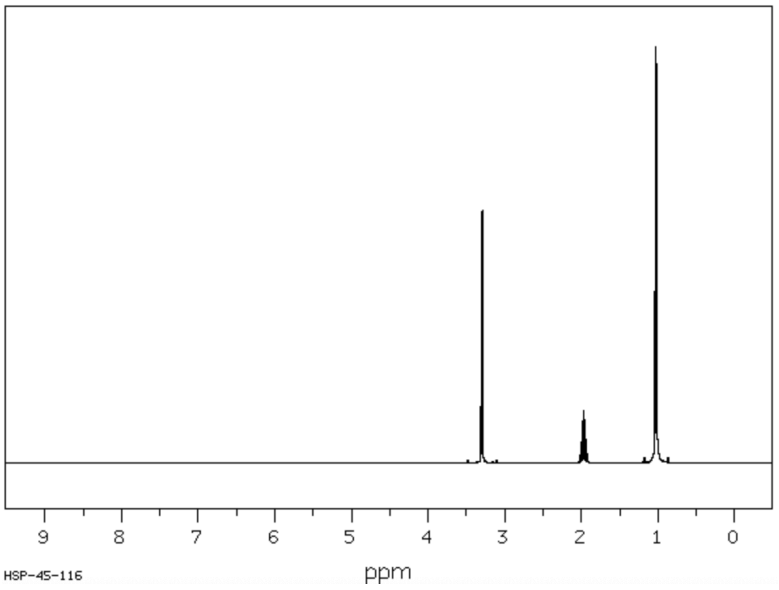
$C_5H_{10}O$

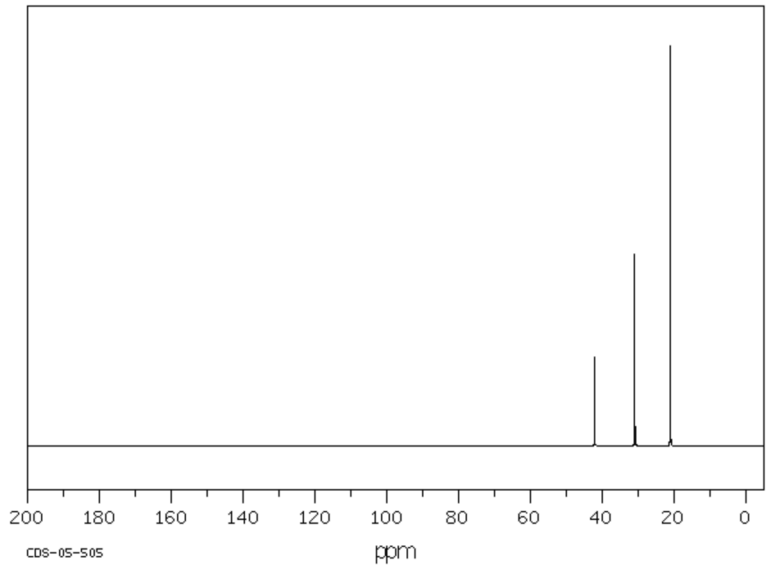


C_4H_6O



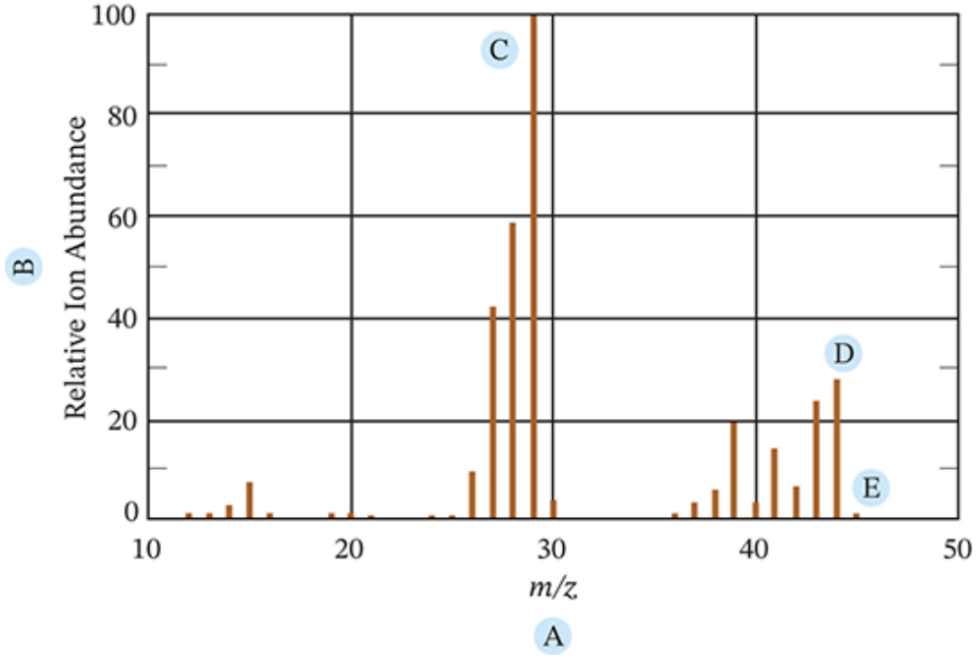
While compiling some results for a paper, your assistant mixes up the ^{1}H NMR and ^{13}C NMR spectra results for various compounds. They give you the following spectra, which they claim match 1-Bromo-2-methylpropane. Are they correct?





Mass Spectrometry:

Anatomy of a mass spec



A:

B:

C:

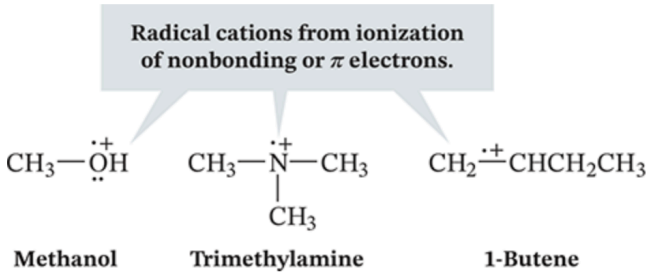
D:

E:

Forming the molecular ion

$$CH_3CH_2CH_3 + e^- \longrightarrow [CH_3CH_2CH_3]^{+\cdot} + 2e^-$$

Another visual/other considerations:



Fragmentation

$$[CH_3CH_2CH_3]^{+\cdot} \rightarrow CH_3\overset{+}{C}H_2 + \cdot CH_3$$
$$[CH_3CH_2CH_3]^{+\cdot} \rightarrow CH_3\dot{C}H_2 + {}^{+}CH_3$$

Putting the reaction together

$$CH_3CH_2CH_3 \xrightarrow{-e^-} CH_3CH_2\overset{+\cdot}{C}H_2CH_3 \longrightarrow CH_3\dot{C}H_2 + \cdot CH_3 \quad (m/z\ 29)$$
or
$$CH_3CH_2\overset{+\cdot}{C}H_2CH_3 \longrightarrow CH_3\dot{C}H_2 + {}^{+}CH_3 \quad (m/z\ 15)$$

Alcohols have a peak at _____ because of_____

Ionization potential:

TABLE 9.3

Ionization Potentials of Selected Molecules

Compound	Ionization Potential (eV)
$CH_3(CH_2)_3NH_2$	8.7
C_6H_6 (benzene)	9.2
C_2H_4	10.5
CH_3OH	10.8
C_2H_6	11.5
CH_4	12.7