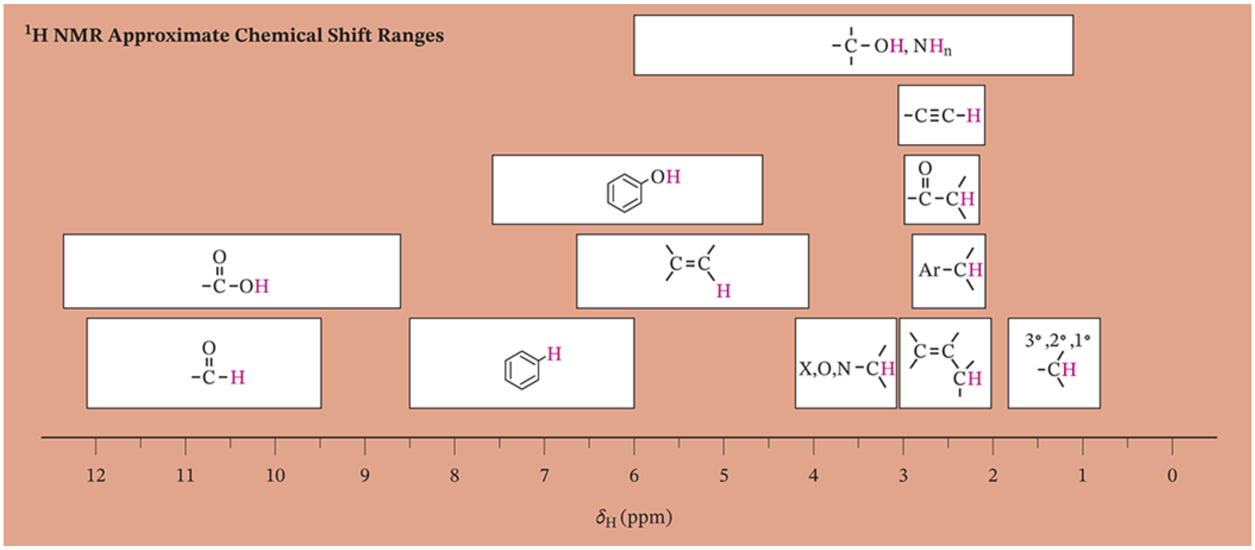
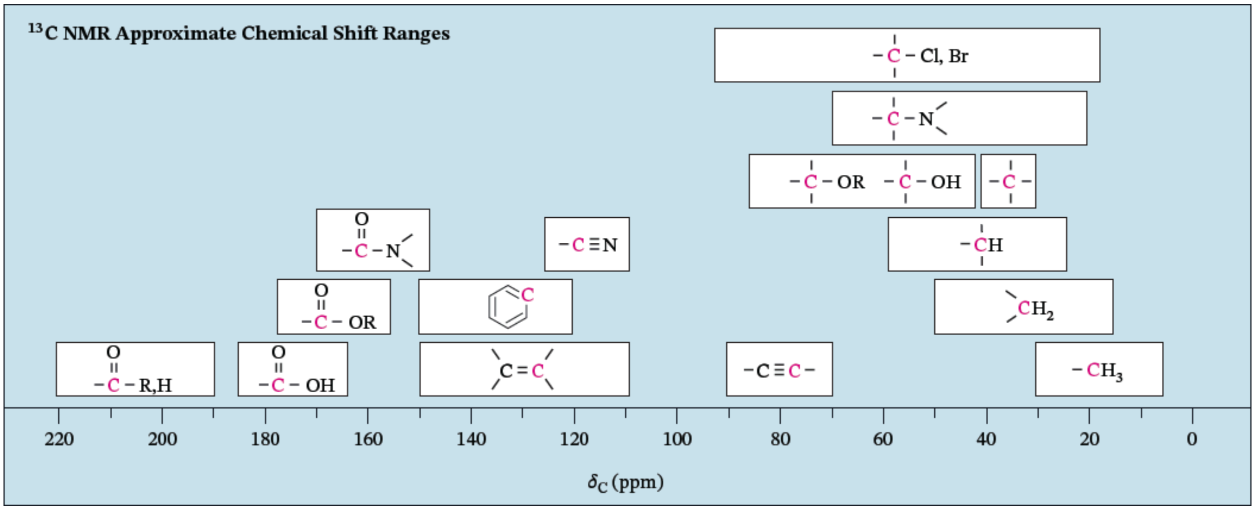
Session 17 Worksheet

Remember these:



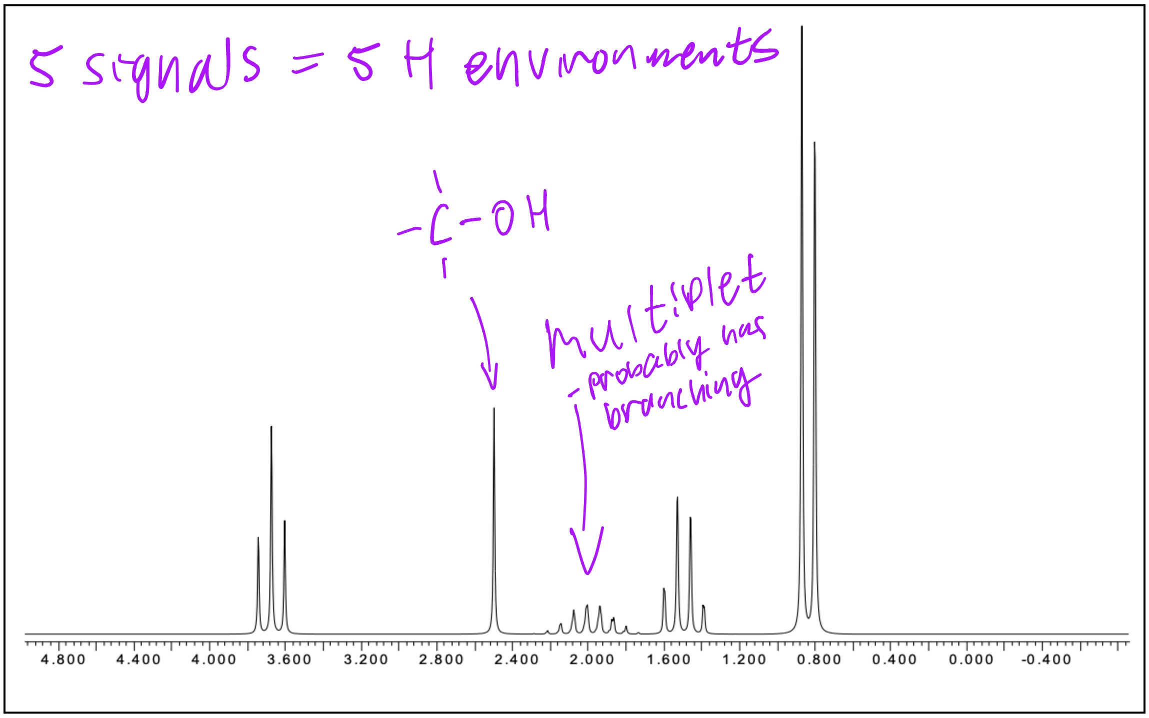


5 carbons

$C_5H_{12}O$

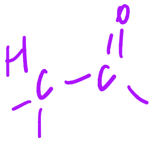
Continuing with ^1H NMR

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



1°, 2°, 3°

Given the molecular formula and signal report, propose a structure



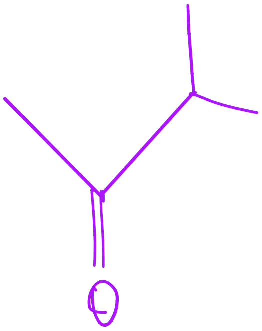
$C_5H_{10}O$

δ = 0.95 ppm (6H, doublet)
δ = 2.10 ppm (3H, singlet)
δ = 2.43 ppm (1H, multiplet)

1°, 2°, 3°
-CH signal
2 of them = (R<)

3 signals = 3 H environments

probably means branching



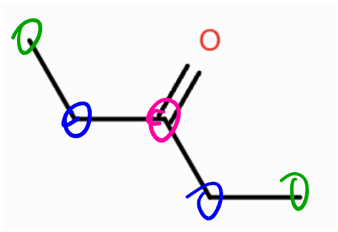
^{13}C NMR:

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

Carbon environments can also have symmetry

^{13}C NMR signal do not have multiplicity, so the signals on ^{13}C NMR look like a straight line

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



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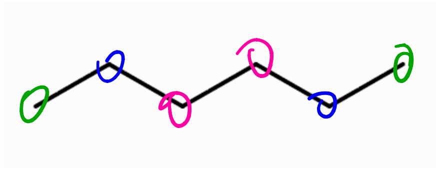

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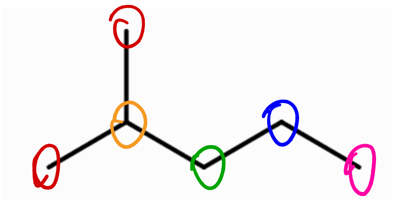

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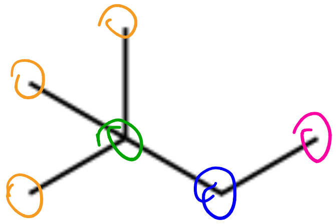
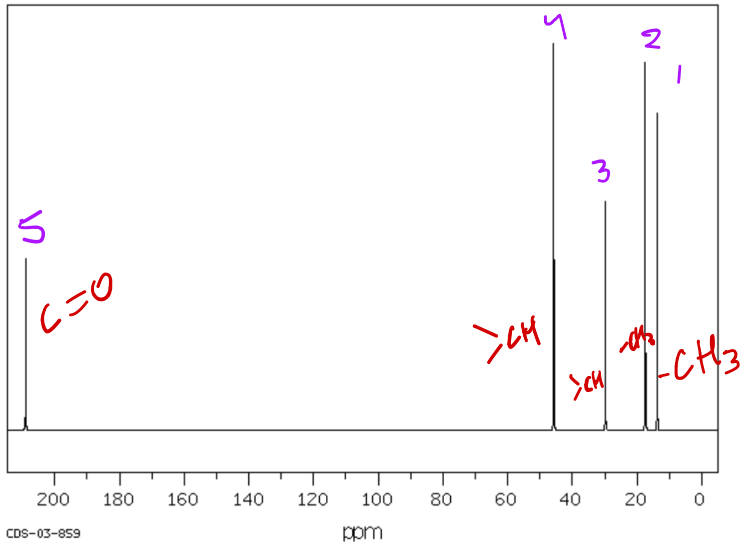


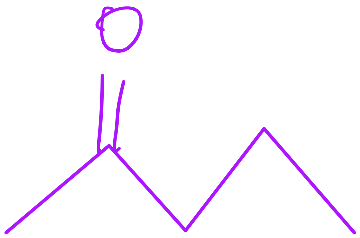
4

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

$C_5H_{10}O$

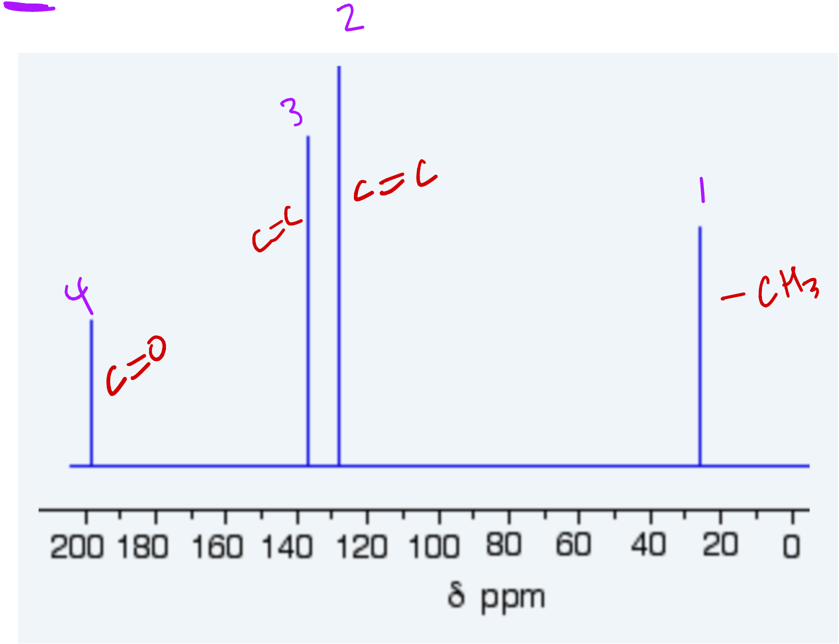
No symmetry

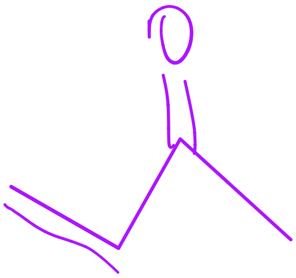




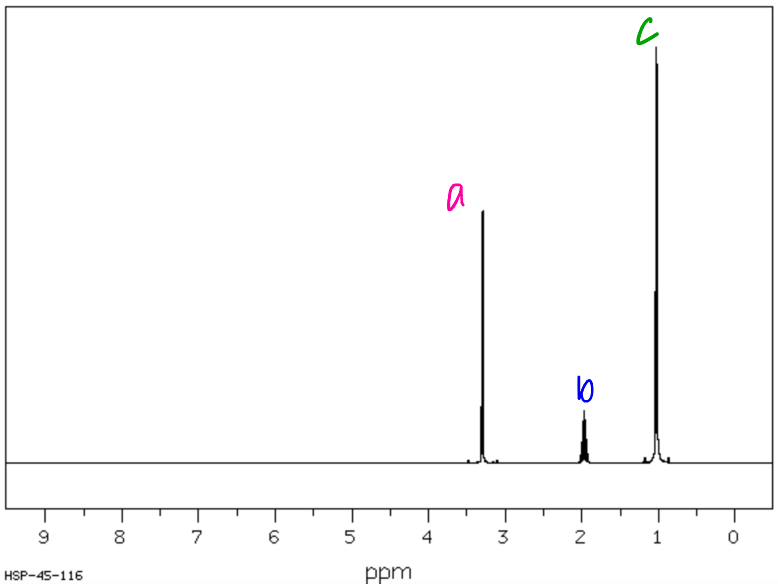
C_4H_6O

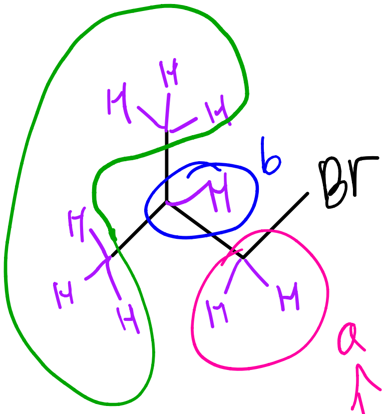
No symmetry





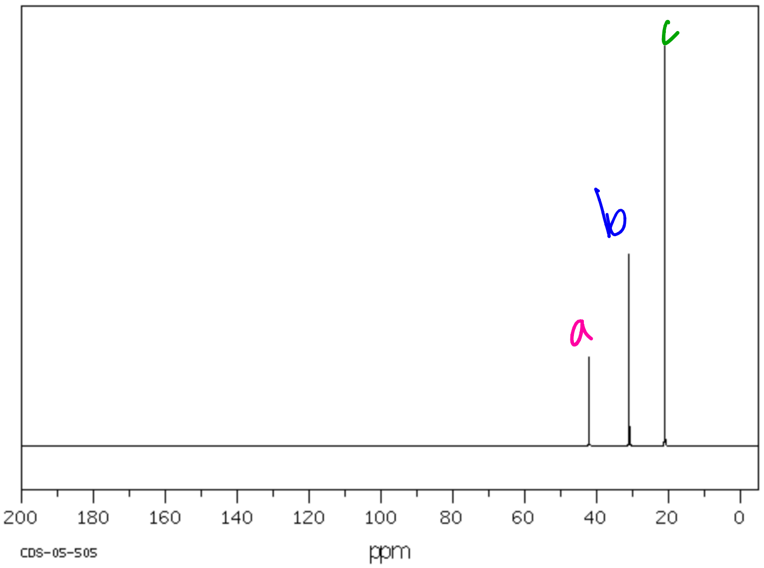
While compiling some results for a paper, your assistant mixes up the ^1H NMR and ^{13}C NMR spectra results for various compounds. They give you the following spectra, which they claim match 1-Bromo-2-methylpropane. Are they correct?

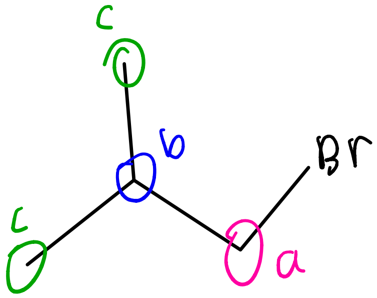




a

more desheilded





requires you to know relative signals

C–Br ≈ 18–92

–CH ≈ 25–59

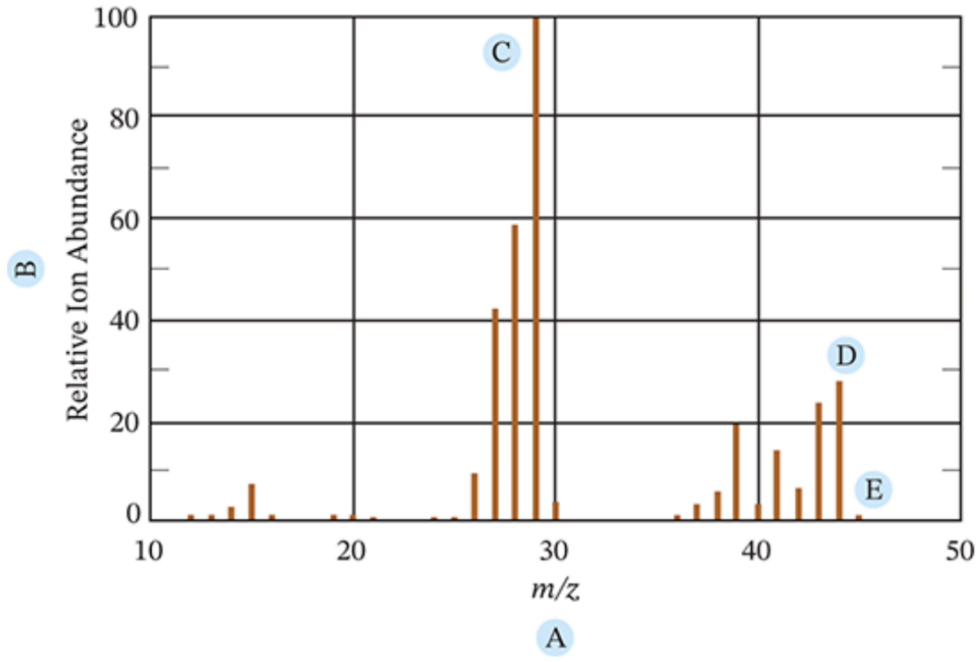
–CH_3 ≈ 5–30

rough estimate

Mass Spectrometry:

Generating, sorting, and detecting various ions in a molecule using high energy e^-

Anatomy of a mass spec



A: Formula weight of each ion

B: abundance of each ion

C: Base peak, the tallest and most abundant ion, usally the easiest fragment formed from the OG compound

D: Molecular ion, represents the closest structure and weight of the original compound

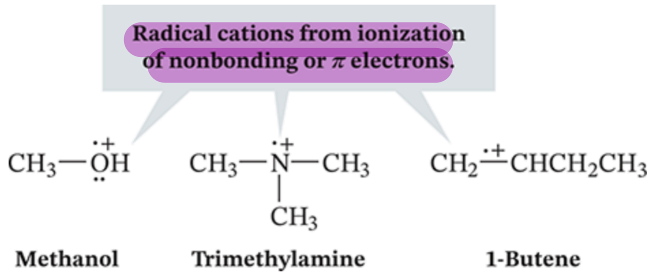
E: Isotope peak, represents isotopes found in a compound

Forming the molecular ion

the molecular ion

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

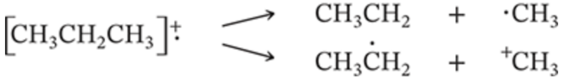
Another visual/other considerations:



Fragmentation

fragmenting

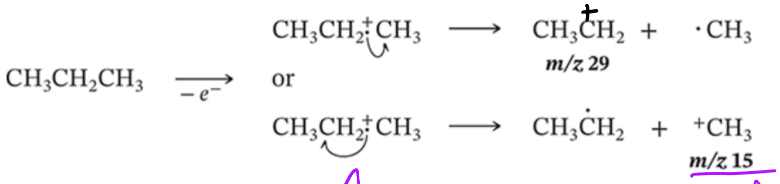
radical cation



radical cation

The radical cation is what gets detected

Putting the reaction together



movement of a radical

weight of ion

Alcohols have a peak at $M^{+\cdot} - 18$ because of loss of H_2O molecule

Ionization potential:

- The amount of energy needed to remove a valence e^- from the molecule

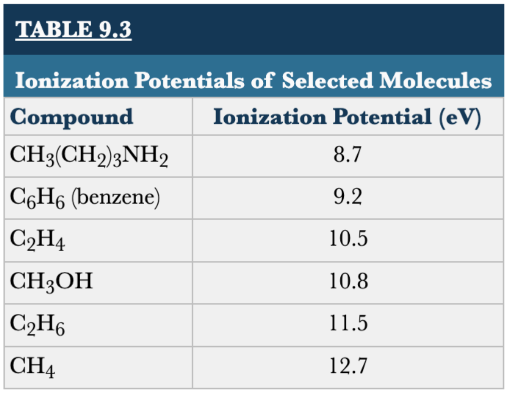


TABLE 9.3

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