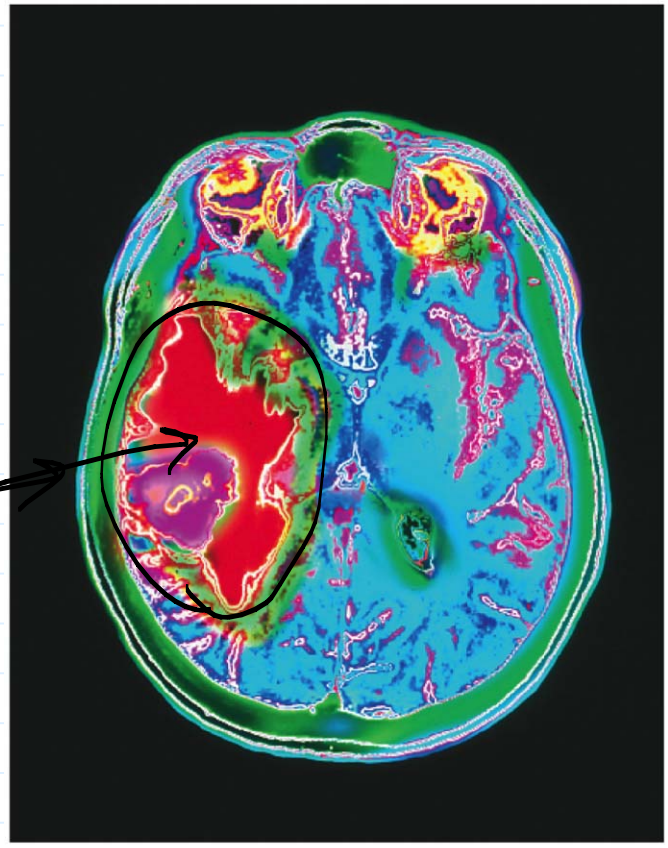
Nuclear Magnetic Resonance (NMR) Spectroscopy

Note Title 3/13/2014

* most important technique for organic chemists.

- uses same technology as MRI
- noninvasive diagnostic tool.

NMR: ^{1}H, ^{13}C, + other "spin-active" nuclei



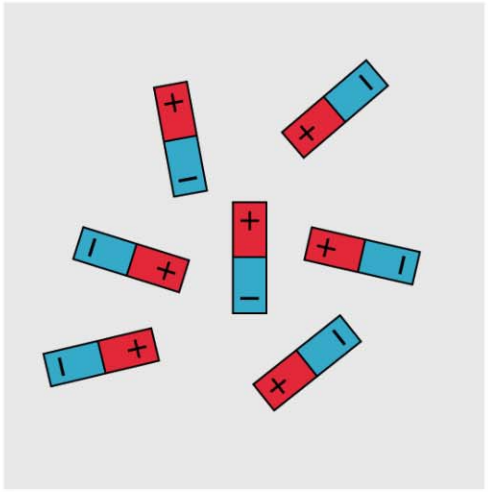
How does it work?

- Detects very low energy transitions of atomic nuclei w/ nuclear spin
  - ↳ Atoms w/ odd number of protons or neutrons (or both)
    - ex: ^{1}H, ~~^{12}C~~, ^{13}C

Spin gives nuclei a magnetic dipole moment.
Spin-active nuclei behave as dipoles.

In presence of external magnetic field, nuclei ≈ bar magnets.

In the absence of an applied magnetic field



In the presence of an applied magnetic field, B_0

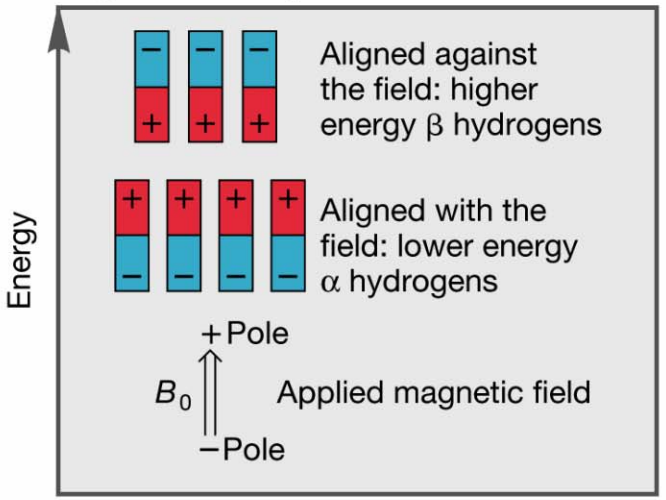
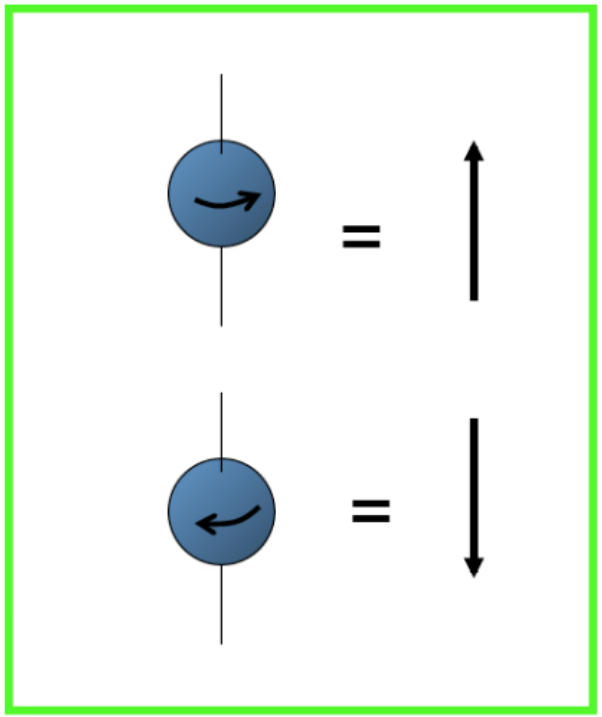
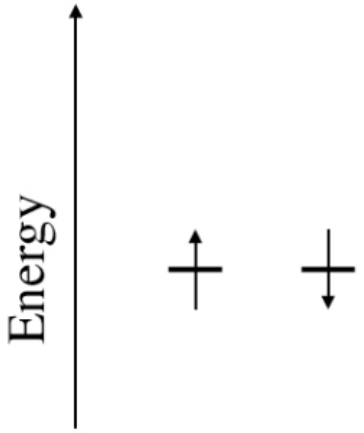
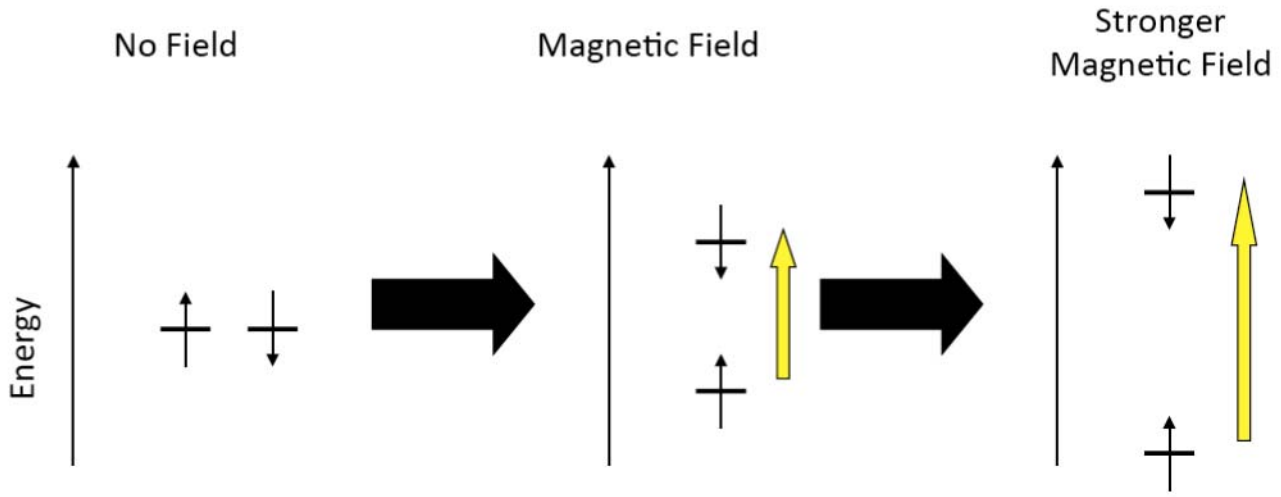


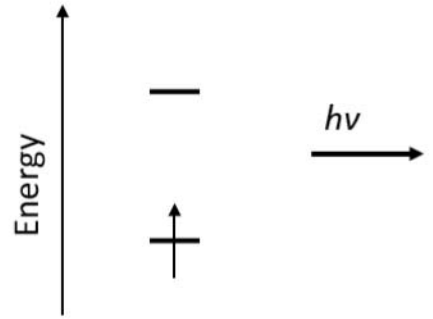
Figure 15.18





In the absence of a magnetic field, both spin states have equal energy





energy of radio waves.

$\Delta E = h\nu$

In a strong magnetic field, the energy level difference corresponds to the energy of radio waves

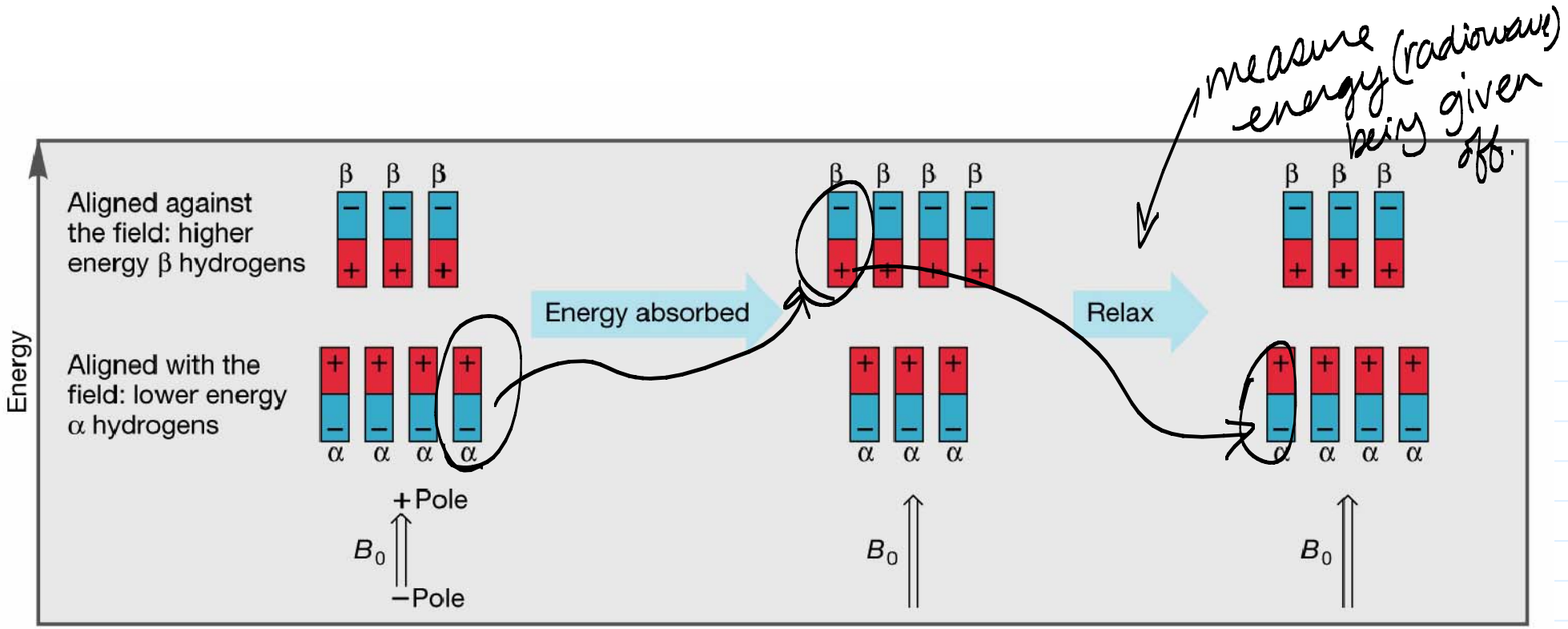
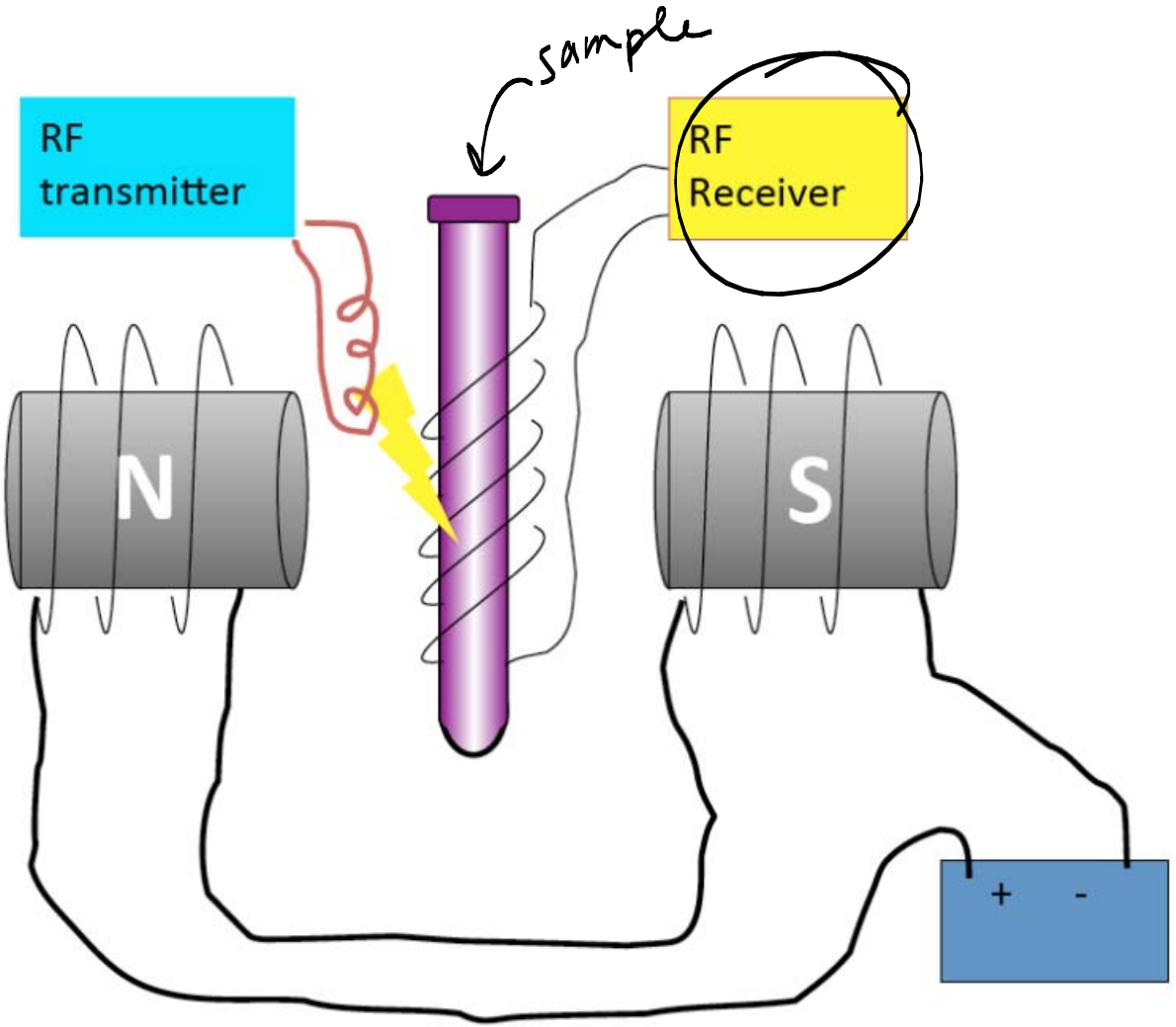


Figure 15.19



Note modern NMRs use superconducting magnets to attain very strong magnetic fields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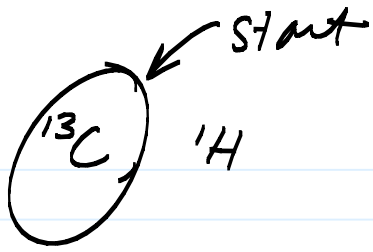
Nuclei that matter in organic chemistry: ^{13}C, ^{1}H



^{13}C NMR

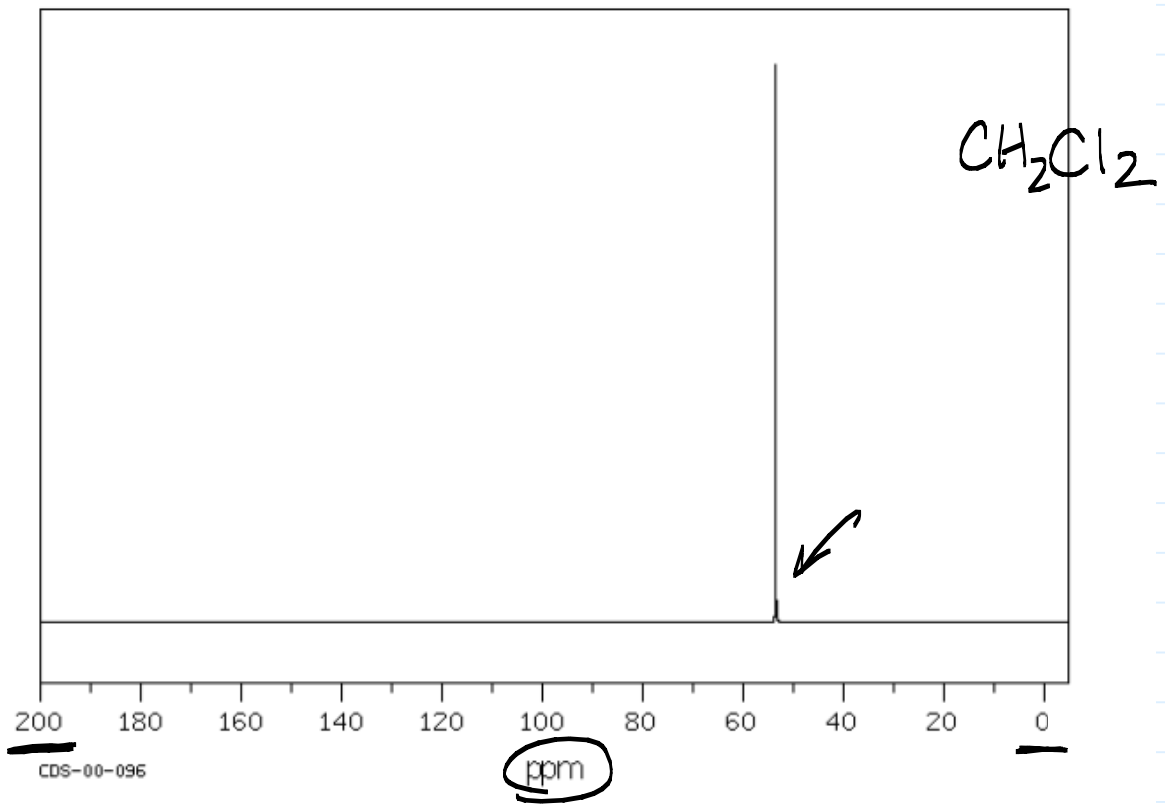
Recall: Most C is ^{12}C (invisible by NMR)

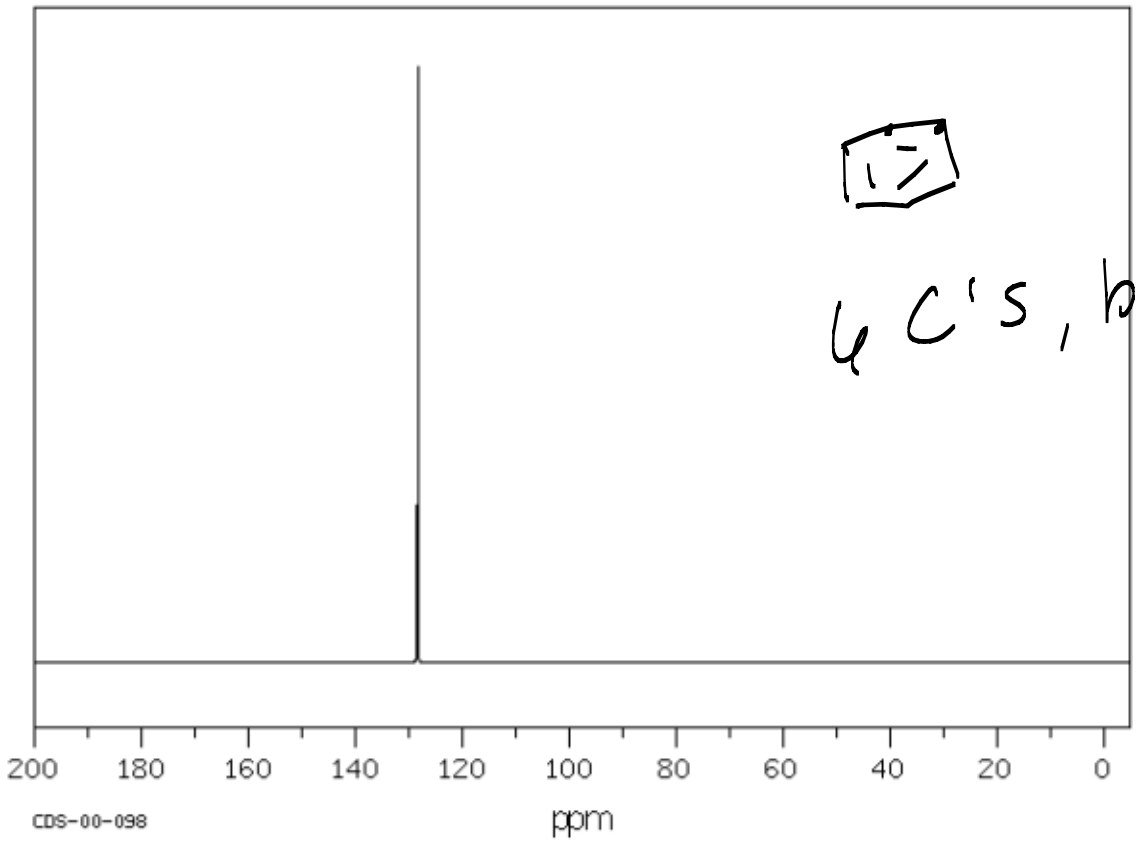
Only ^{13}C is spin-active (~1%)

What does it tell you?

Tells you how many types of C are in your molecule (& what types)

Different types of C appear at different frequencies b/c the e-s around nuclei "shield" them from external magnetic field.


CH_2Cl_2
200
180
160
140
120
100
80
60
40
20
0
ppm
CDS-00-096



6 C's, but only 1 type

↓

1 peak in ^{13}C NMR

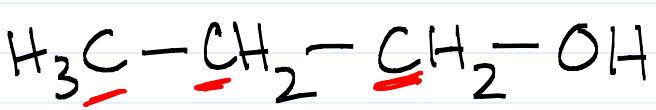
Solving the Structure of an Unknown... (or 2)...

Molecular Formula: $C_3H_8O \longrightarrow$ HCF: C_3H_8 — Sat. Alkane: $C_3H_{(2n+2)}$, $n = 3$

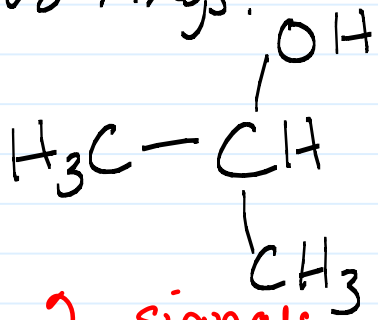
Ø degrees of unsaturation.

↓

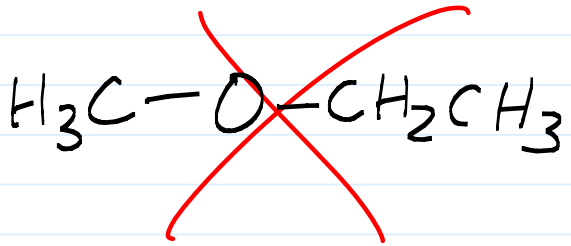
No π bonds, No rings.



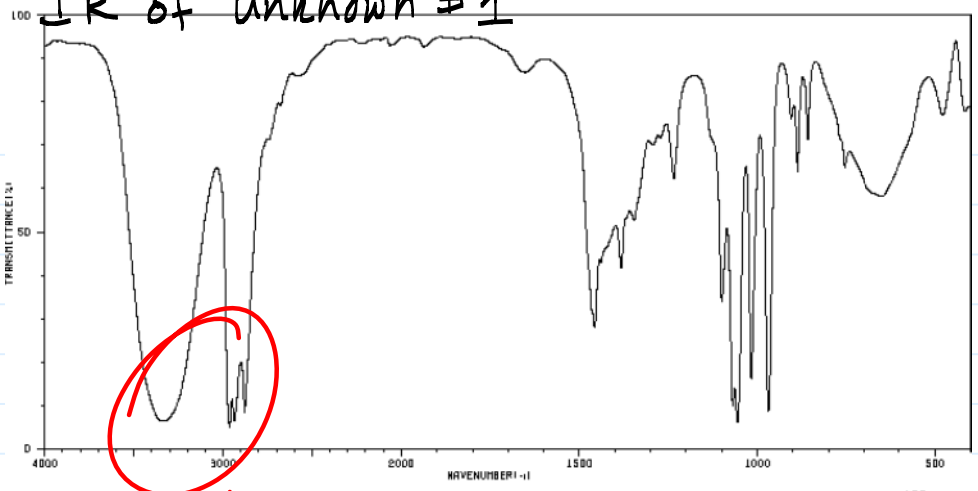
3 ^{13}C signals



2 signals in ^{13}C NMR



IR of unknown #1

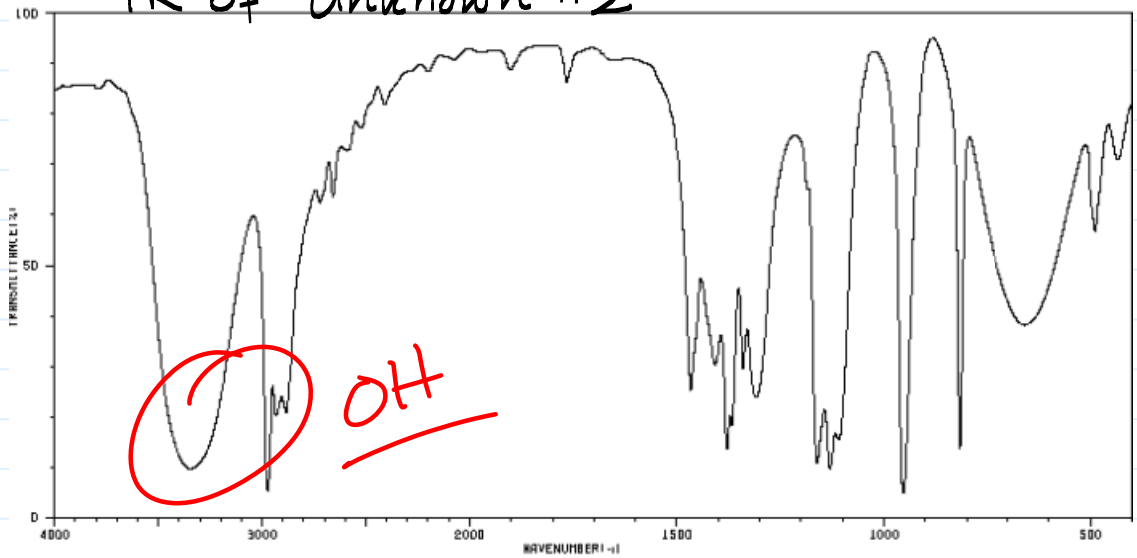


OH

Both unknowns are alcohols.

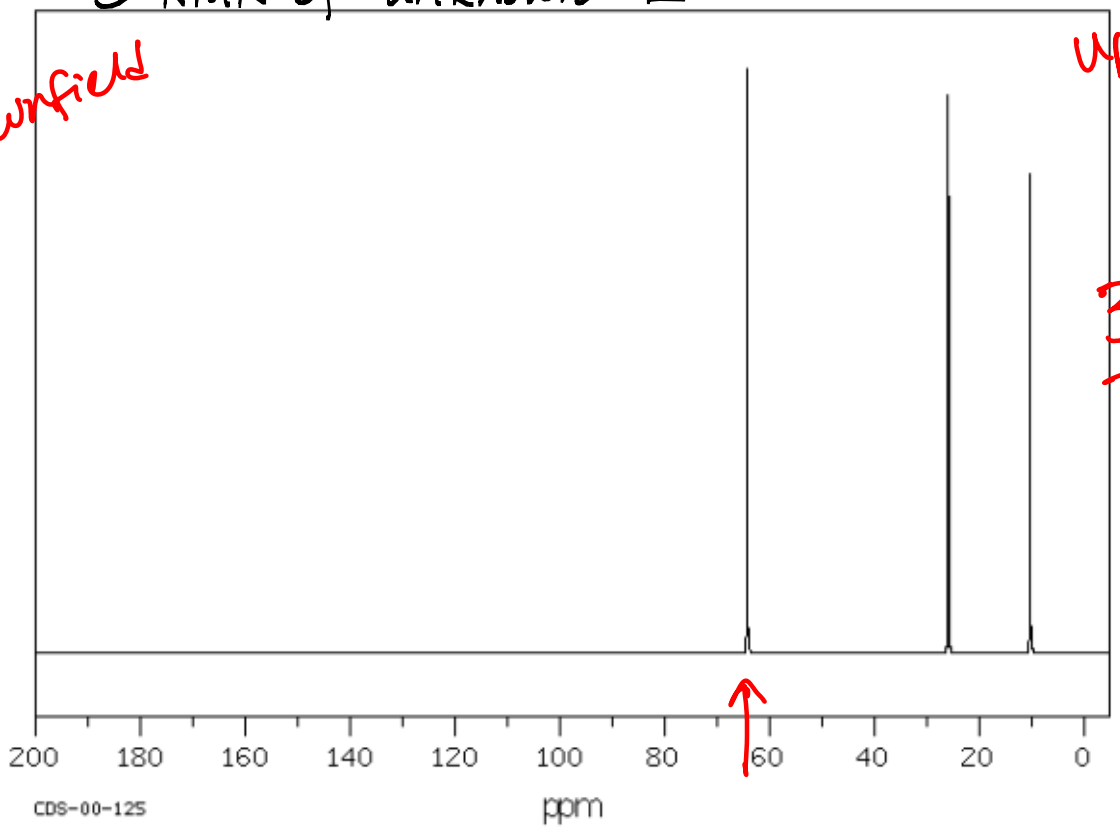
→ Ruled out ether structure.

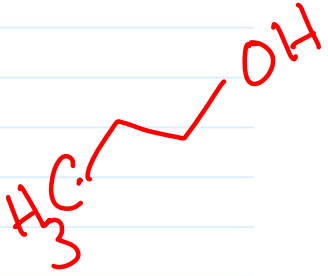
IR of unknown #2



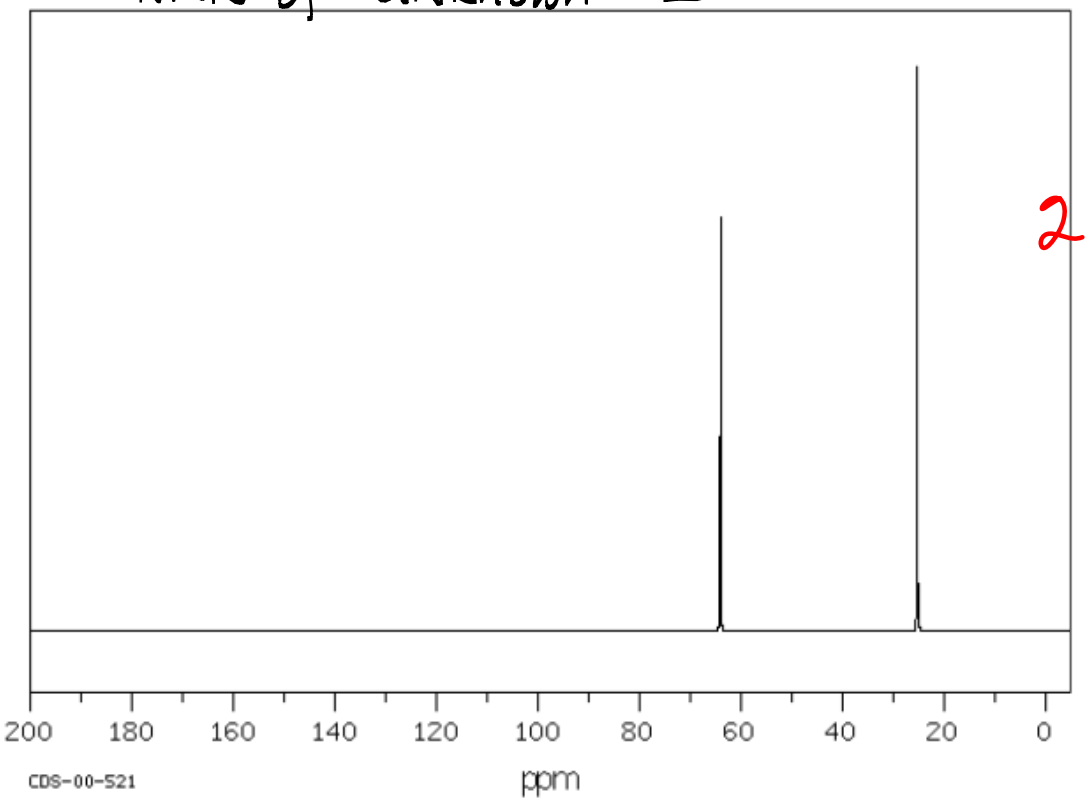
OH

^{13}C NMR of Unknown #1

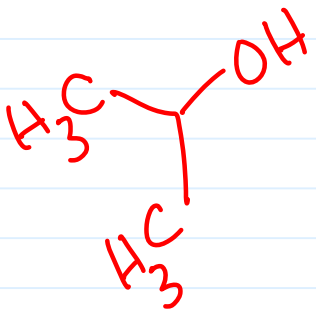




^{13}C NMR of Unknown #2

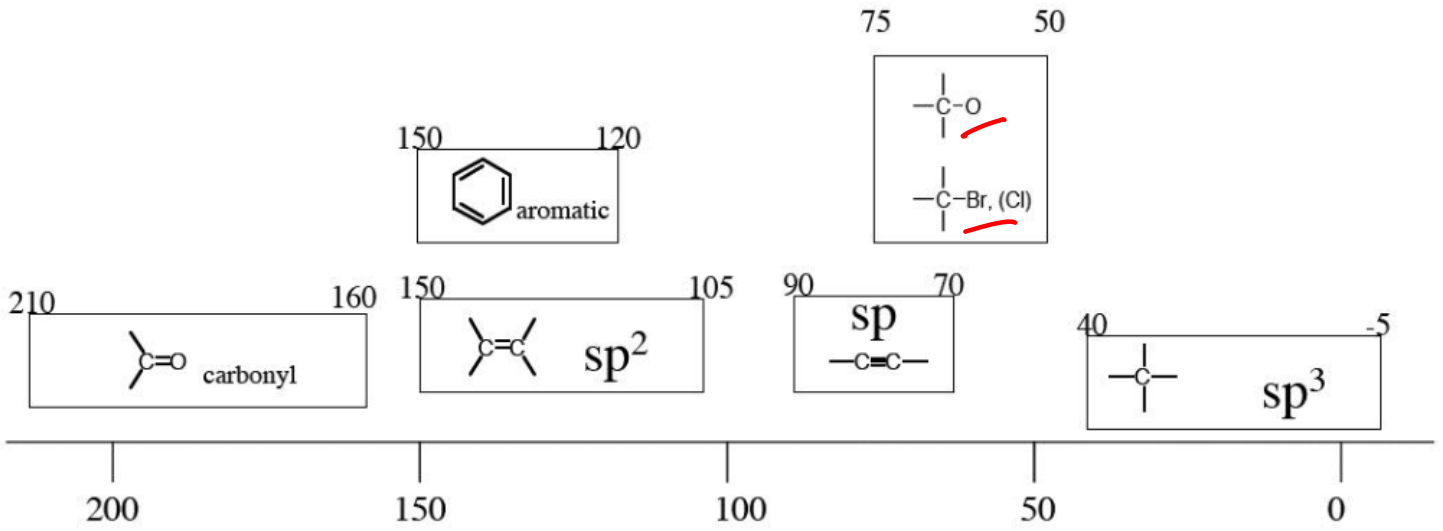


2 signals



Where a peak appears (0–200 ppm) = CHEMICAL SHIFT

- hybridization of C
- electronegativity of attached atom(s)



Midterm 1 :

Average : 183 /250

A : 220 - 250

B : 183 - 219

C : 121 - 182