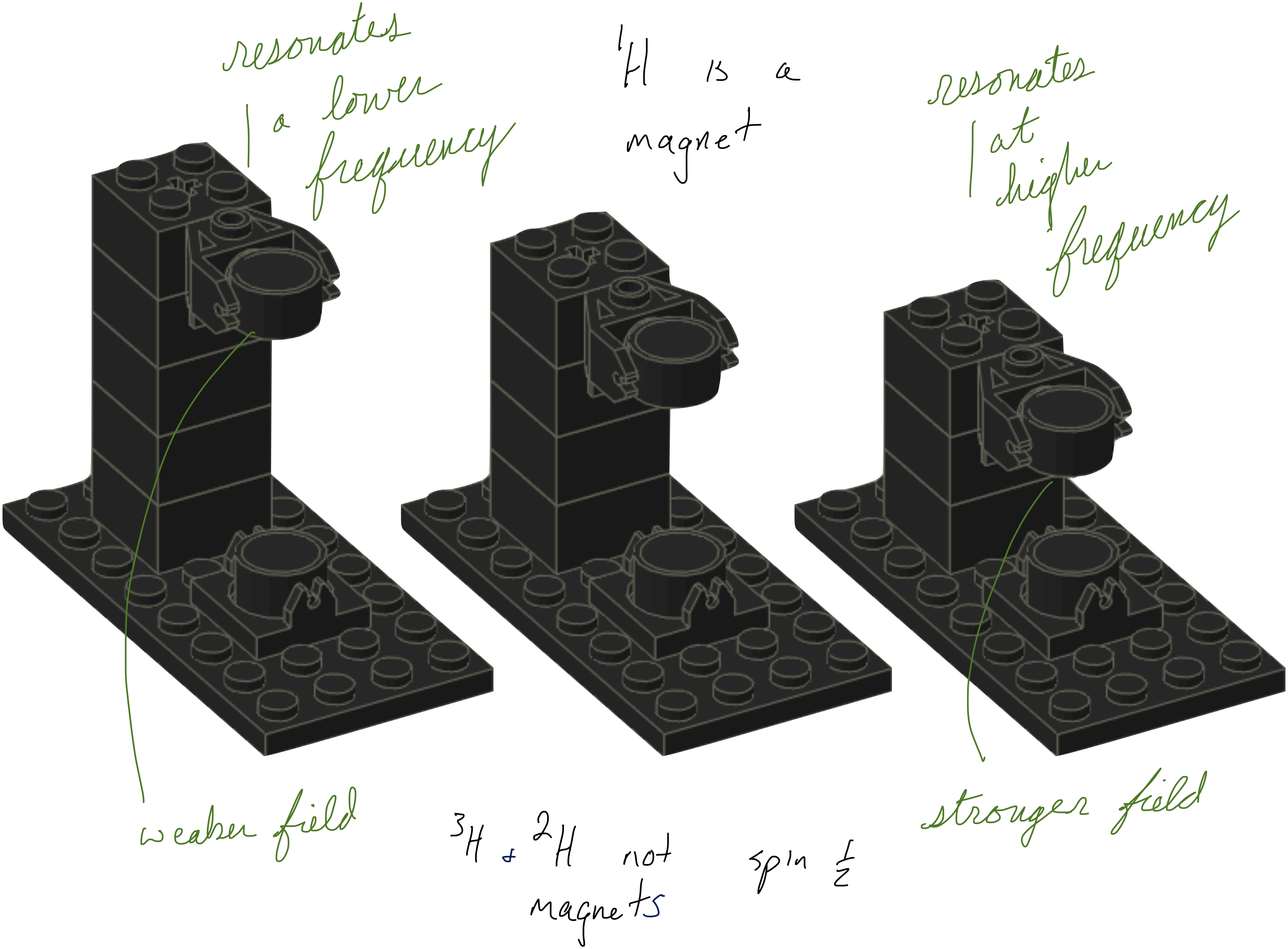
Magnets placed in a magnetic field align with the magnetic field.
When perturbed the magnets will "resonate".
The frequency of the resonance depends on the strength of the magnetic fields

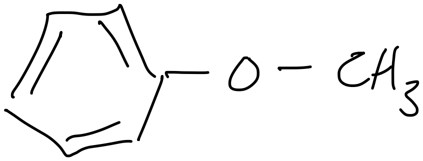

resonates
a lower
frequency
^1H is a
magnet
resonates
at
higher
frequency
weaker field
^3H & ^2H not
magnets
spin $\frac{1}{2}$
stronger field

a super conducting wire with e^- going round and round

~1.4 T magnet will cause ^1H to align & resonante at ~ 60,000,000 Hz

900 MHz, (21.2 T) NMR Magnet at HWB-NMR, Birmingham, UK
https://en.wikipedia.org/wiki/Nuclear_magnetic_resonance#/media/File:HWB-NMR_-_900MHz_-_21.2_Tesla.jpg

sample experiences a uniform magnetic field

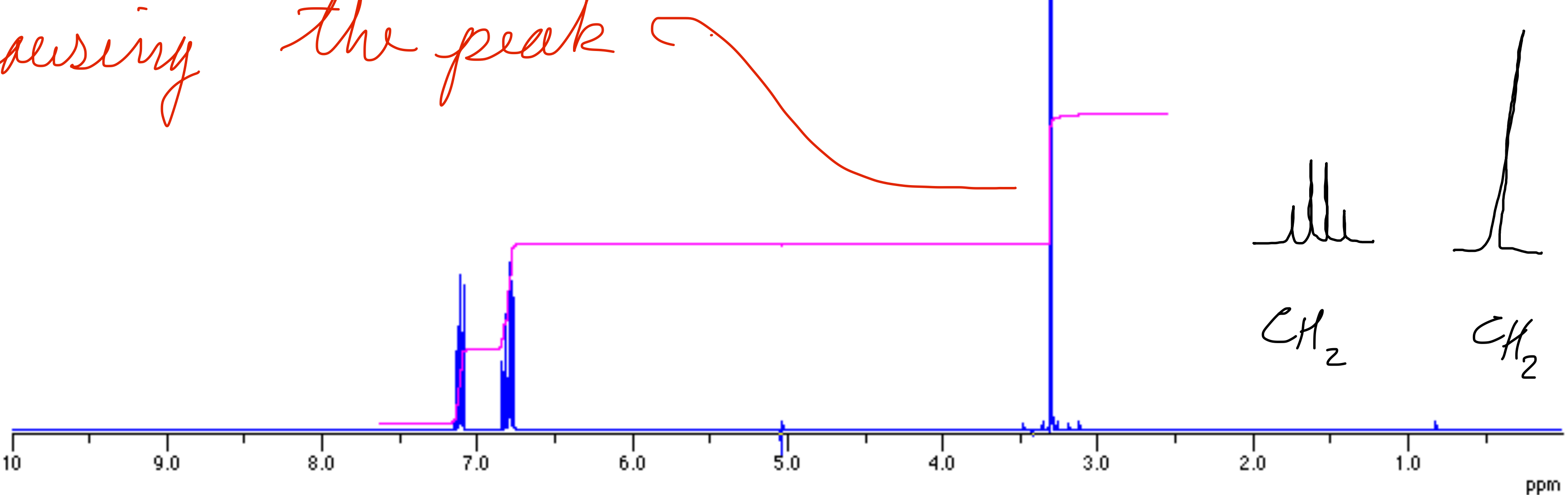


The # of peaks is related to the number of different H's in our molecule.

relative #'s of ^1H atoms causing the peak

The chemical environment

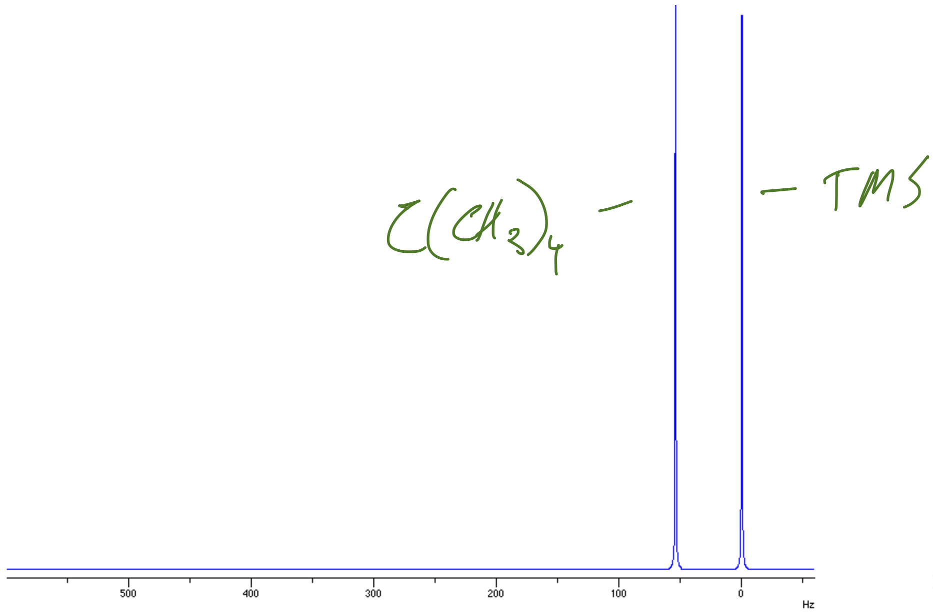
The # of H atoms on neighboring C, N, or O atoms



magnetic field varies based on position

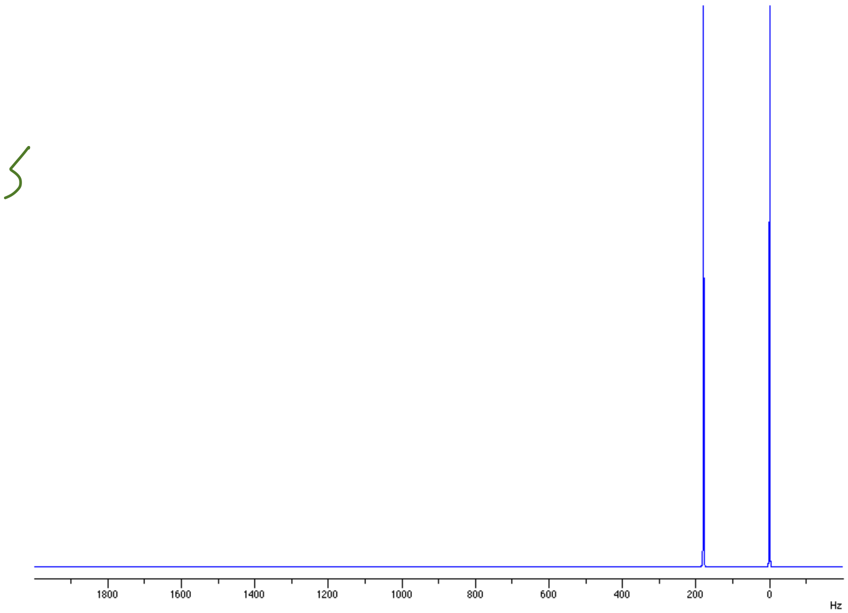
www.radiologyinfo.org

Magnetic Resonance Imaging H_2O



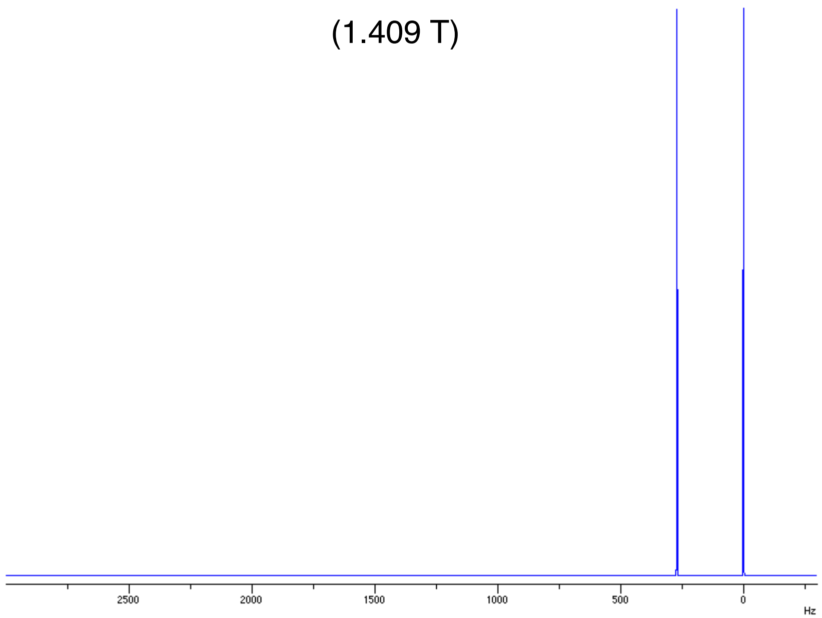
+ 60,000,000 Hz (60 MHz)

(1.409 T)



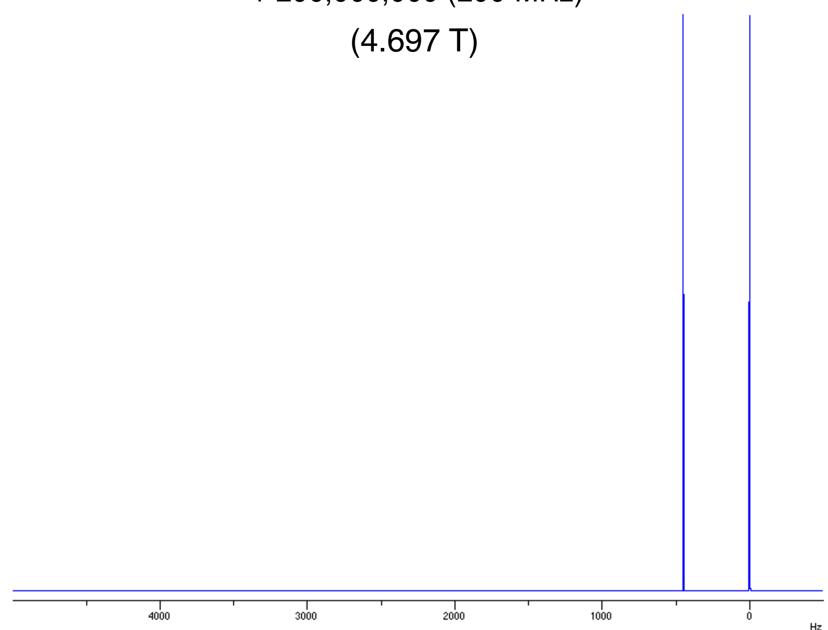
+ 200,000,000 (200 MHz)

(4.697 T)



+300,000,000 Hz (300 MHz)

(7.046 T)



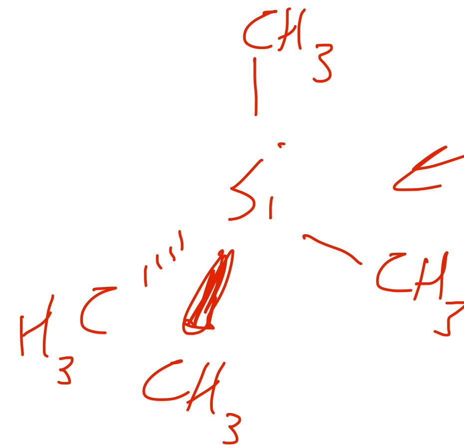
+ 500,000,000 Hz (500 MHz)

(11.743 T)

$$\delta \text{ ppm} = \frac{\nu_{(peak)}\text{Hz} - \nu_{(TMS)}\text{Hz}}{\nu_{(TMS)}\text{MHz}}$$

reference molecule

TMS = tetramethyl silane



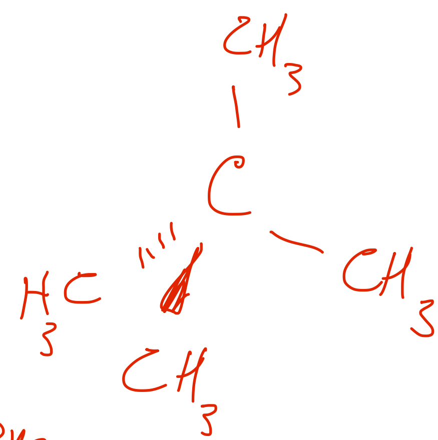
0 ppm

1.409 T magnet TMS resonanates

at 60,000,000 Hz

neopentane resonates at

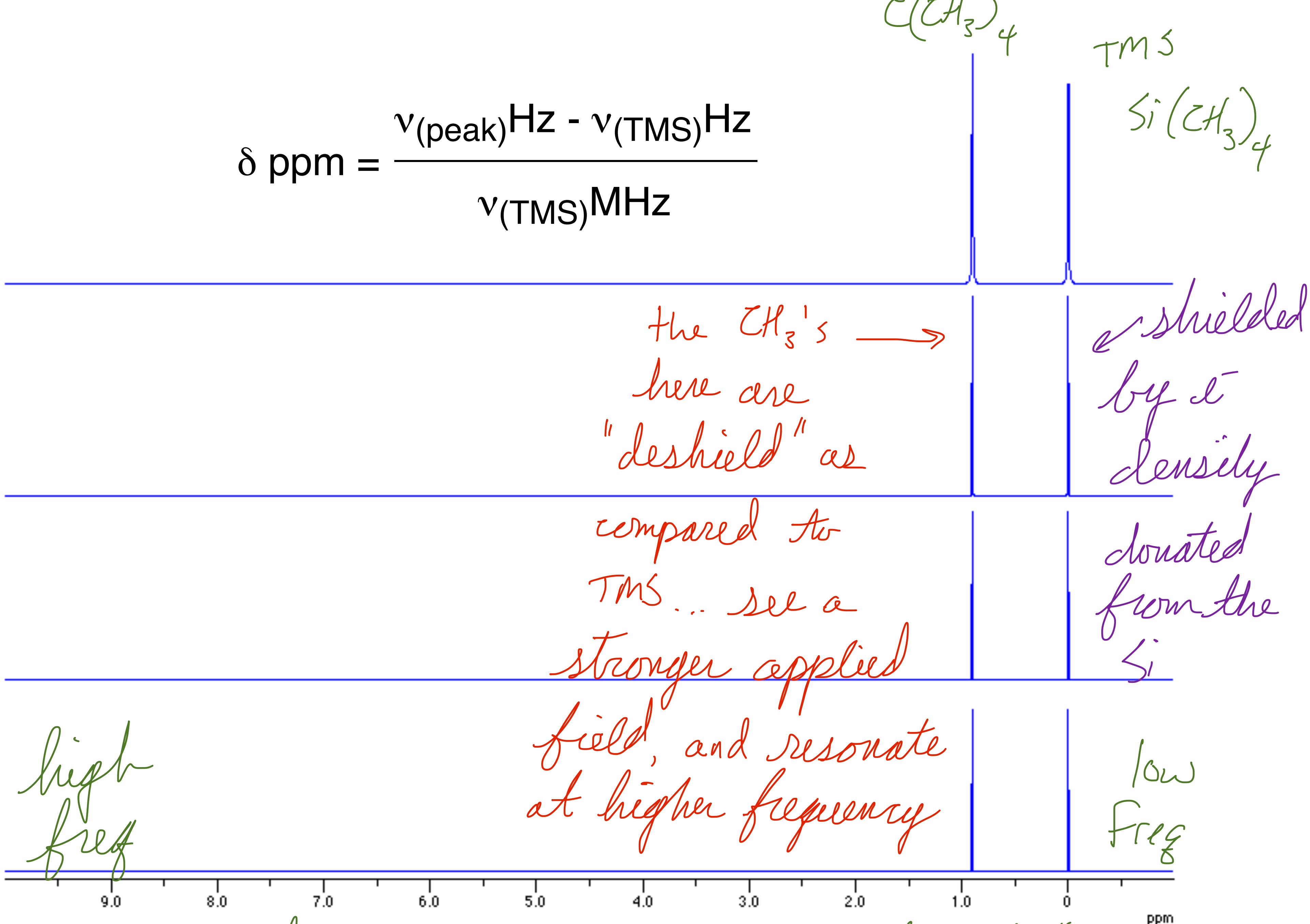
60,000,054 Hz



0.9 ppm

$$\frac{(60{,}000{,}054 - 60{,}000{,}000)\text{Hz}}{60 \text{ MHz}} = 0.9 \text{ ppm}$$

$$\delta \text{ ppm} = \frac{\nu_{(peak)}\text{Hz} - \nu_{(TMS)}\text{Hz}}{\nu_{(TMS)}\text{MHz}}$$



for historical reasons its "backwards"

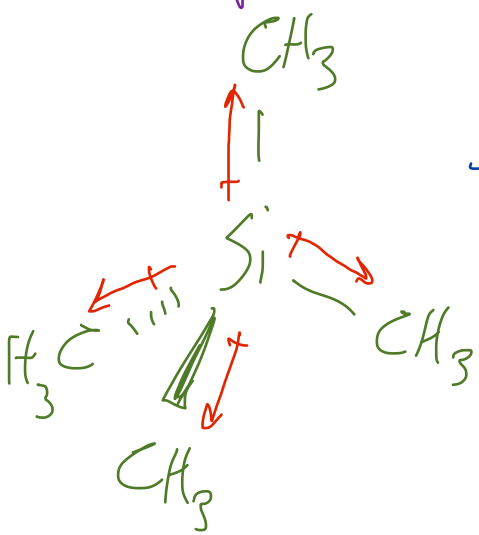
shielding causes these H's to "see" a weaker field & thus resonate at a lower freq

What gives rise to differences in chemical shift?

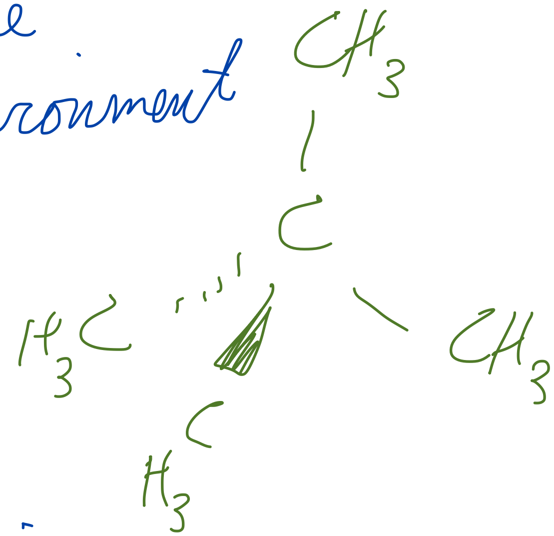
position in NMR spectrum

Why do the H's of tetramethylsilane resonate at a different frequency than 2,2-dimethylpropane?

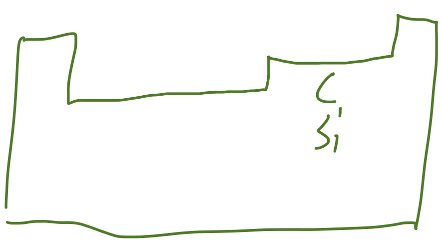
these H are in a more e^- rich environment



vs



these moving e^-'s are creating a magnetic field which shields the H's from the applied field



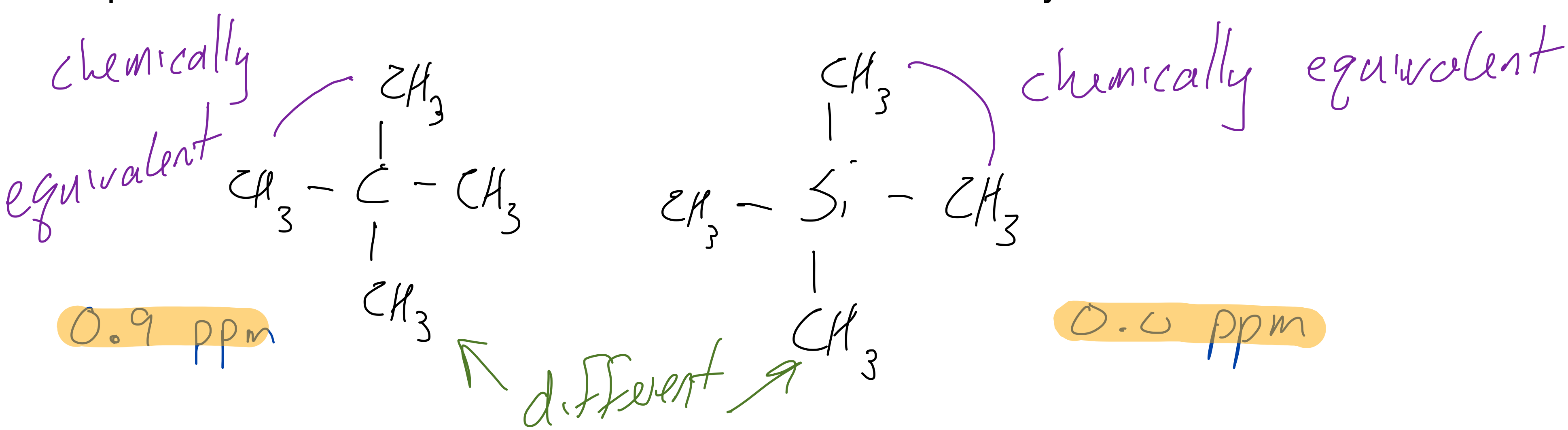
When placed in a magnetic field magnets will align with the applied field.

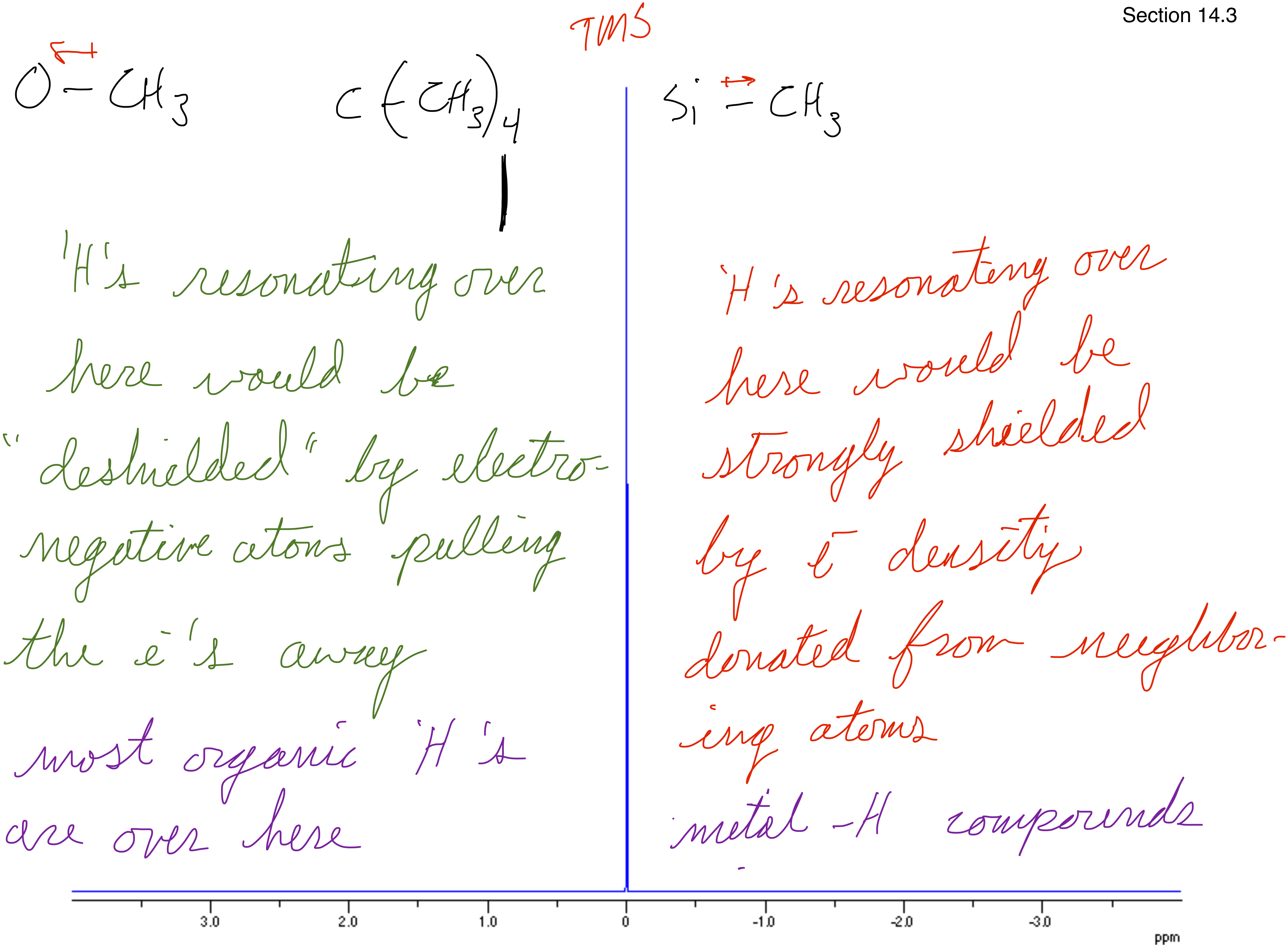
When perturbed magnets will resonate until they return to their equilibrium position.

The frequency of the resonance is determined by the strength of the magnetic field.

Chemically inequivalent H atoms will usually exist in different magnetic environments and will, thus, be magnetically inequivalent and resonate at different frequencies. The position of the peaks relative to the position of a reference peak is referred to as their chemical shift.

Electronegative atoms deshield ^{1}H atoms. Deshielded ^{1}H atoms close to electronegative atoms experience a stronger applied field and resonate at higher frequencies as compared to well shielded ^{1}H atoms like those of tetramethylsilane.




TMS
O–CH3
C(CH3)4
Si–CH3
1H's resonating over here would be "deshielded" by electronegative atoms pulling the e⁻'s away
most organic 1H's are over here
1H's resonating over here would be strongly shielded by e⁻ density donated from neighboring atoms
metal–H compounds
3.0
2.0
1.0
0
-1.0
-2.0
-3.0
ppm

ethyl propionate

4 peaks means
4 sets of inequivalent
^1H's

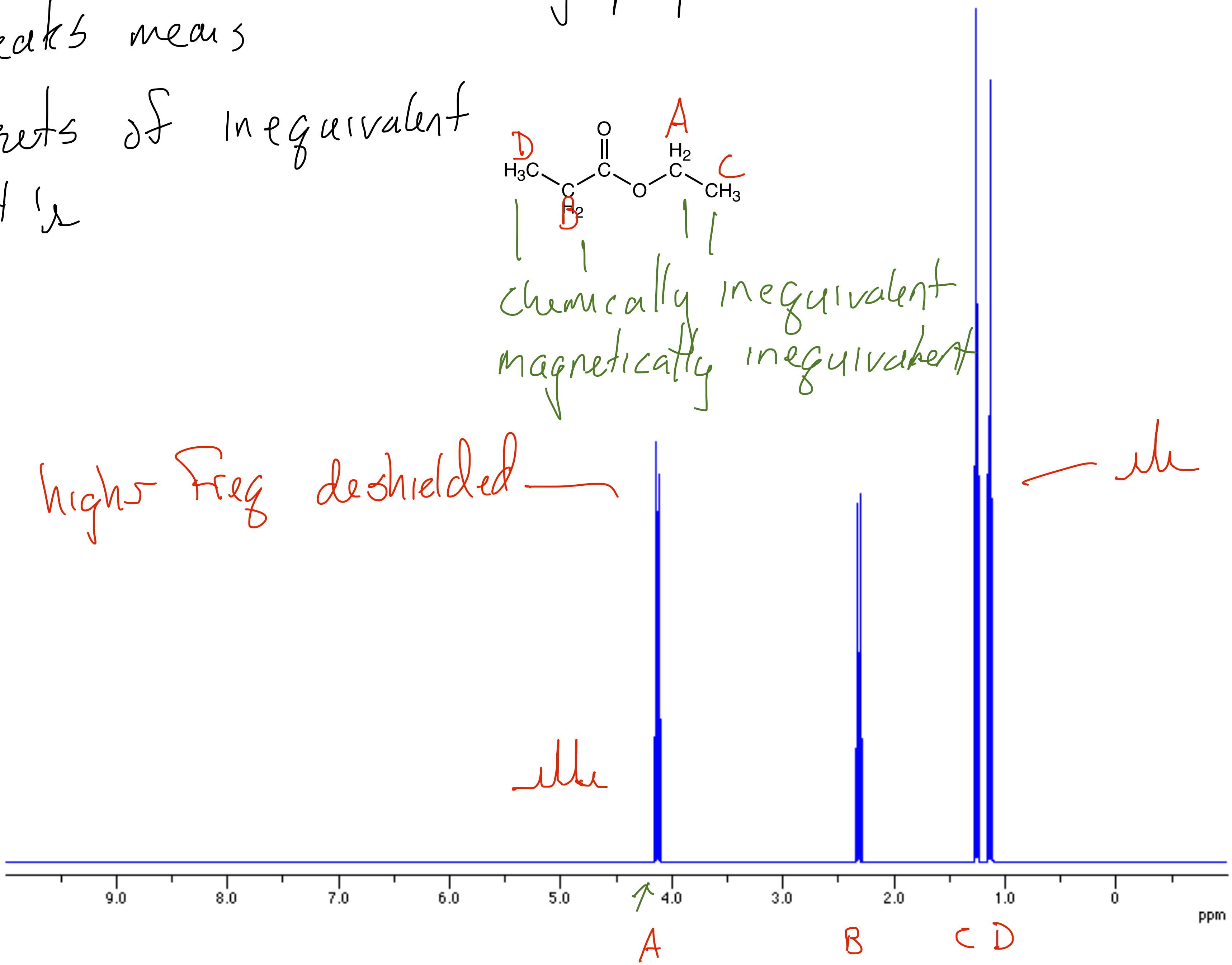
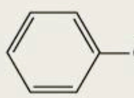


Table 14.1 Approximate Values of Chemical Shifts for ^1H NMR[a]

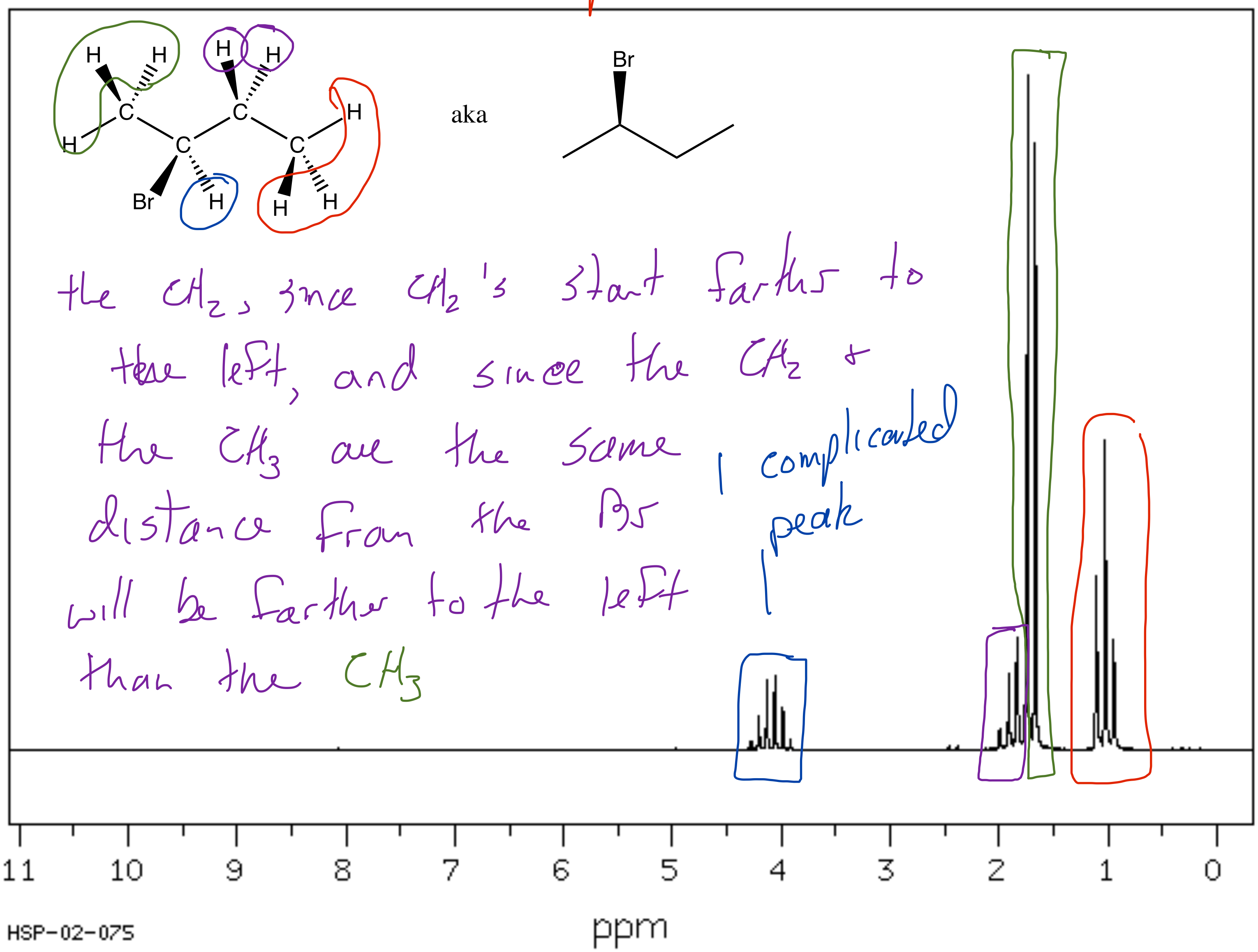
Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0	 $-H$	6.5–8
$-CH_3$	0.9	$-C(=O)-H$	9.0–10
$-CH_2-$	1.3	$I-C-H$	2.5–4
$-CH-$ (with one further bond)	1.4	$Br-C-H$	2.5–4
$-C=C-CH_3$	1.7	$Cl-C-H$	3–4
$-C(=O)-CH_3$	2.1	$F-C-H$	4–4.5
 $-CH_3$	2.3	RNH_2	Variable, 1.5–4
$-C\equiv C-H$	2.4	ROH	Variable, 2–5
$R-O-CH_3$	3.3	$ArOH$	Variable, 4–7
$R-C(R)=CH_2$	4.7	$-C(=O)-OH$	Variable, 10–12
$R-C(R)=C(R)-H$	5.3	$-C(=O)-NH_2$	Variable, 5–8

[a]The values are approximate because they are affected by neighboring substituents.

π bonds create a magnetic field that reinforces the external field

O is deshielding CH_3 so CH_3 resonates at higher frequency

4 peaks



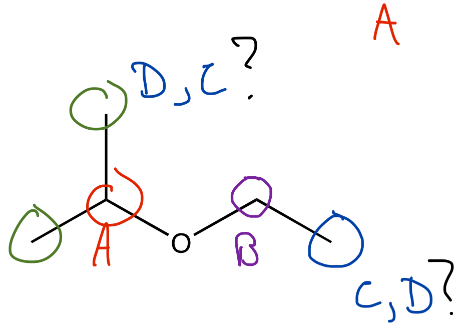
the CH_2, since CH_2's start farther to the left, and since the CH_2 & the CH_3 are the same distance from the Br will be farther to the left than the CH_3

1 complicated peak

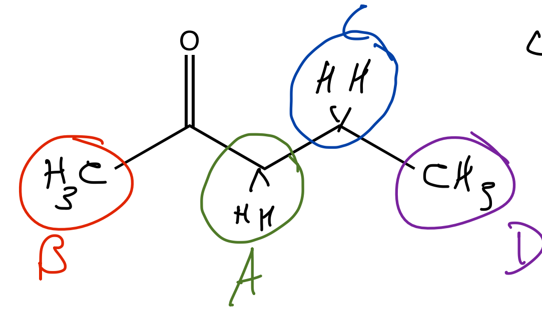
https://sdbs.db.aist.go.jp/sdbs/cgi-bin/landingpage?sdbsno=500

chemically inequivalent = magnetically inequivalent most of the time

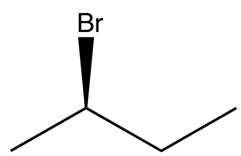
peaks

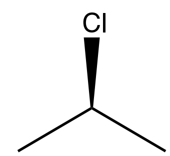


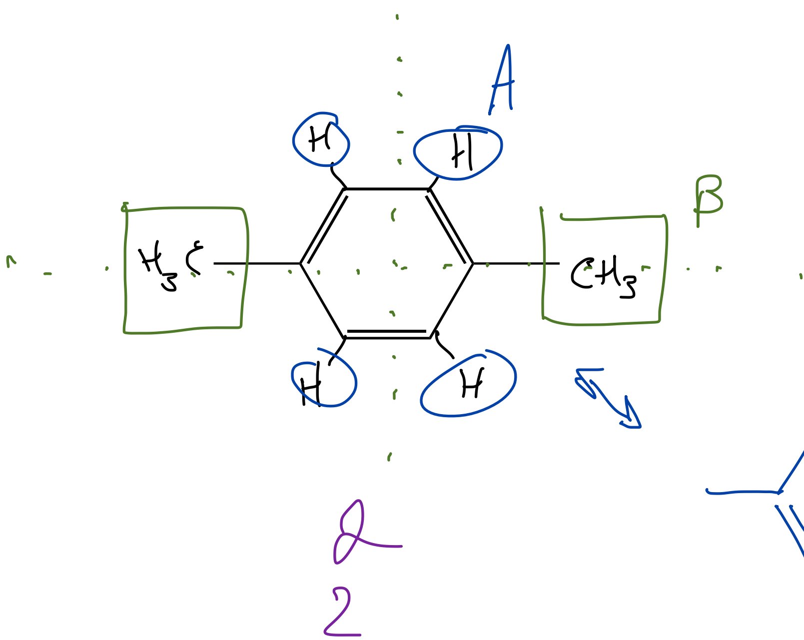
3 4

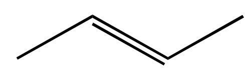


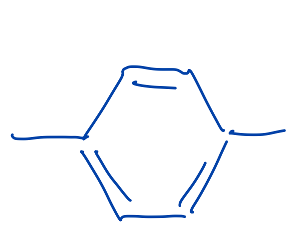
4 5











Number of different types of H atoms

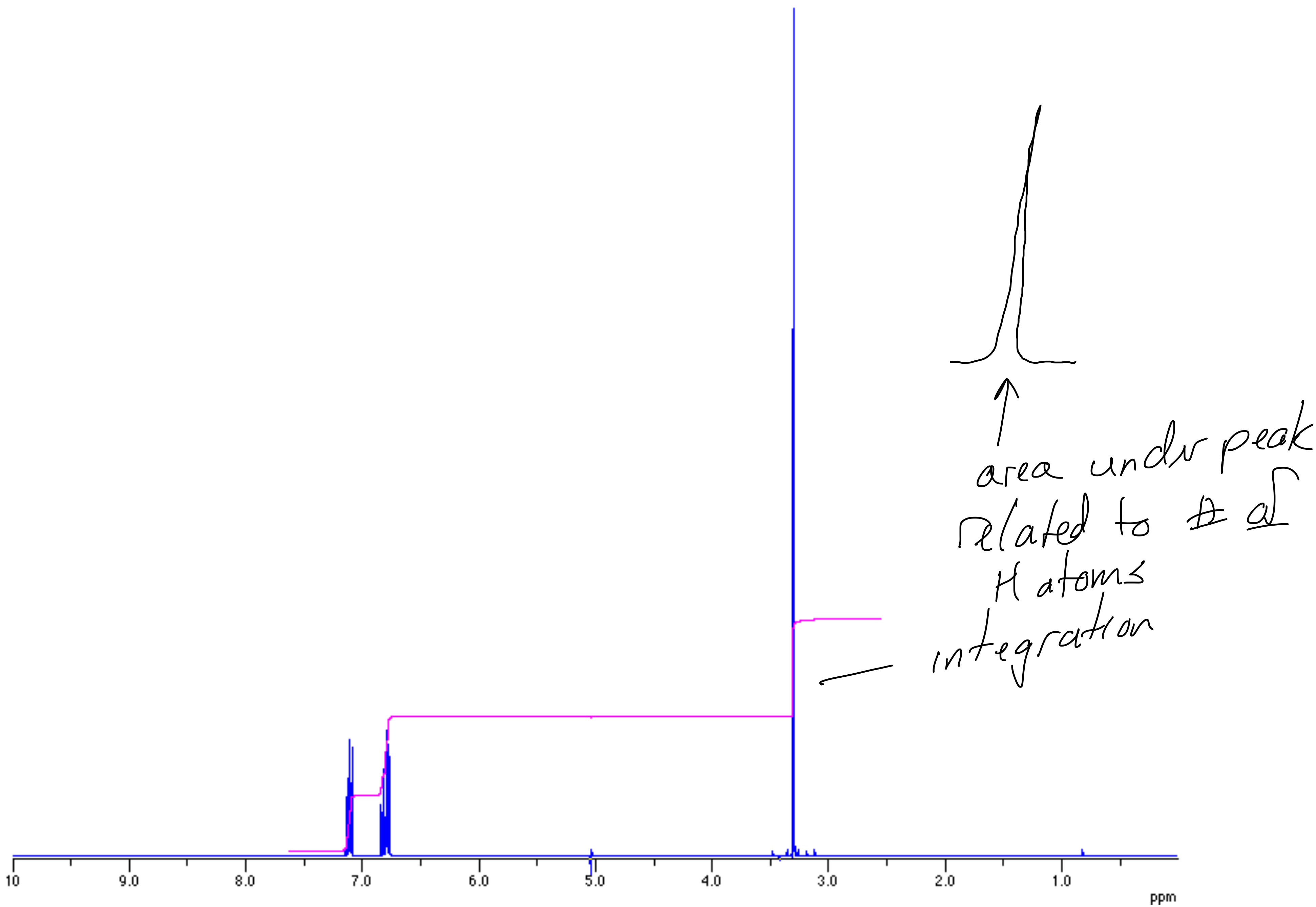
# of peaks

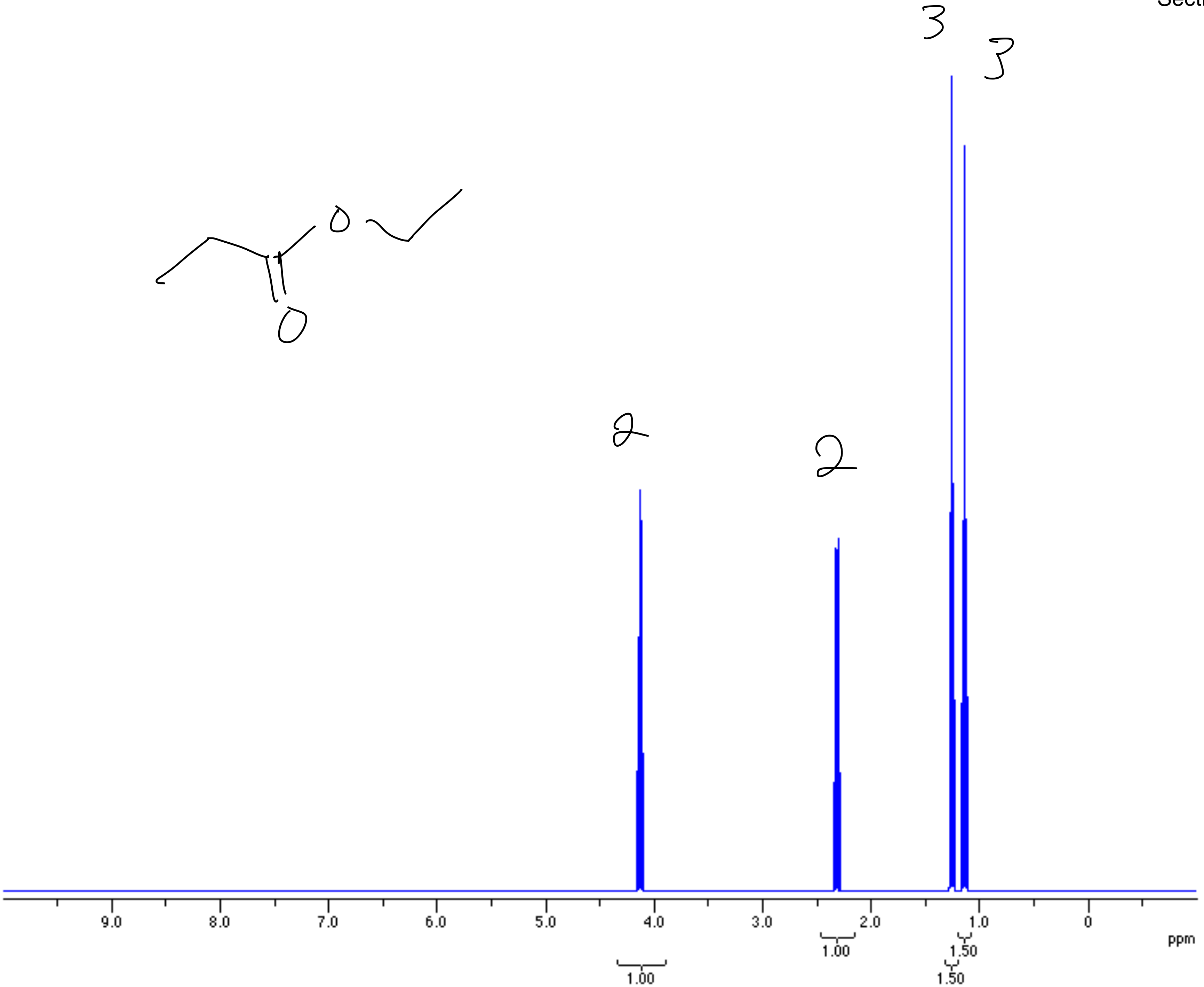
Chemical environments of the H atoms

will determine their chemical shift

to the left ... near eneg atoms

to the left near = bonds


area undr peak
related to # of
H atoms
integration
10
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm

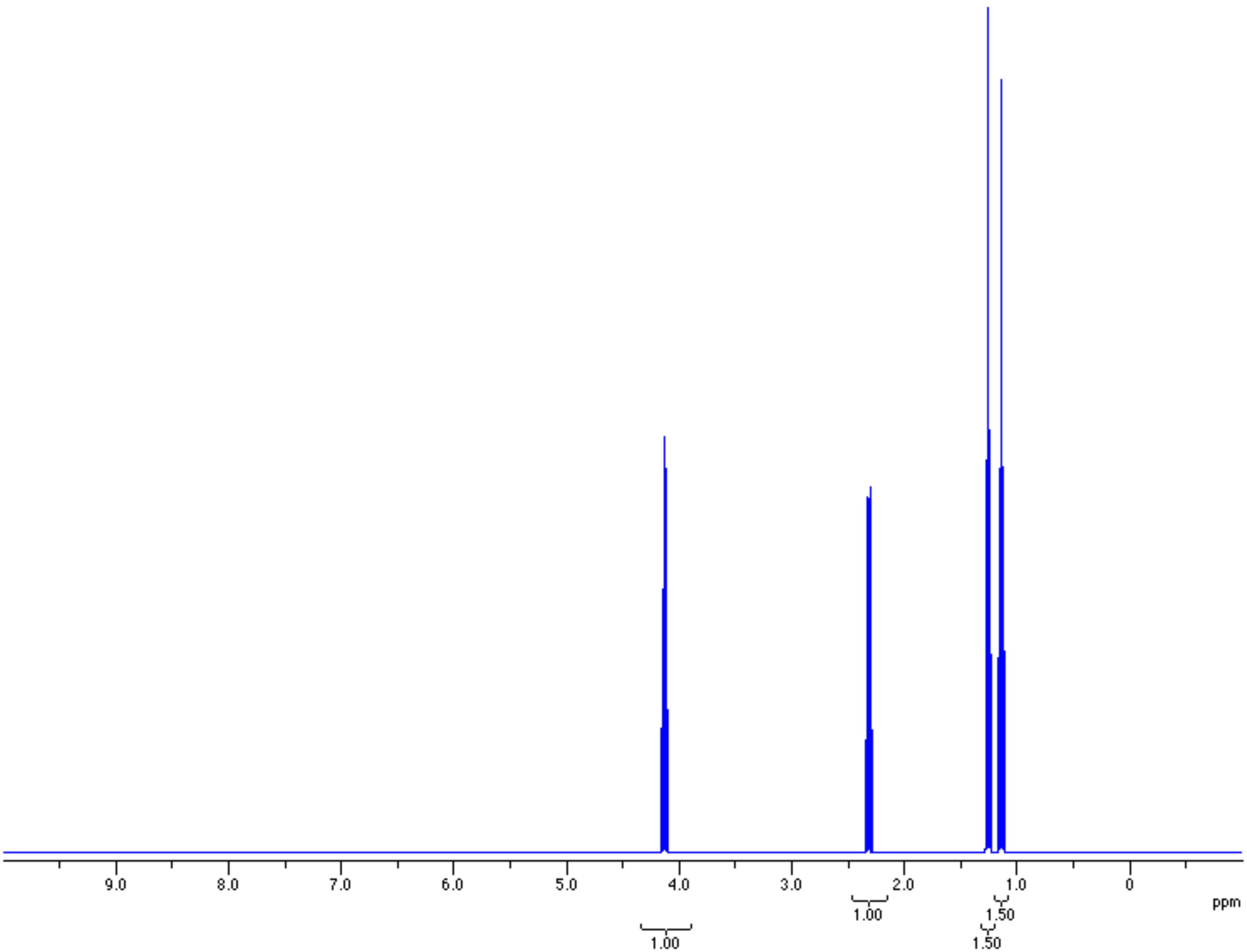


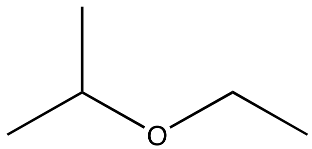
3
3
2
2
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
ppm
1.00
1.00
1.50
1.50

Number of different types of H atoms

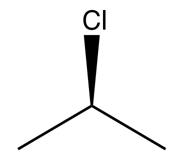
Chemical environments of the H atoms

How many of each type of H atom

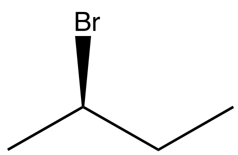

9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
ppm
1.00
1.50
1.00
1.50



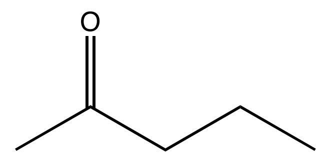
O



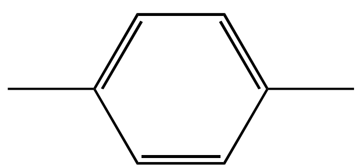
Cl

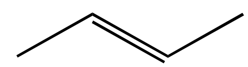


Br



O





Number of different types of H atoms

Chemical environments of the H atoms

How many of each type of H atom

How many H atoms neighbor each different type of H atom