نووي مغناطيس

Nuclear Magnetic Resonance Spectroscopy

UV – VIS

e⁻ exitation
absorbtion
qualitative quantitative

- qualitative only
- λ micro waves نهاية الـ
  radio waves

الهدف

analyzing spectrum in compound (qualitatively) < no. of H / no. of C

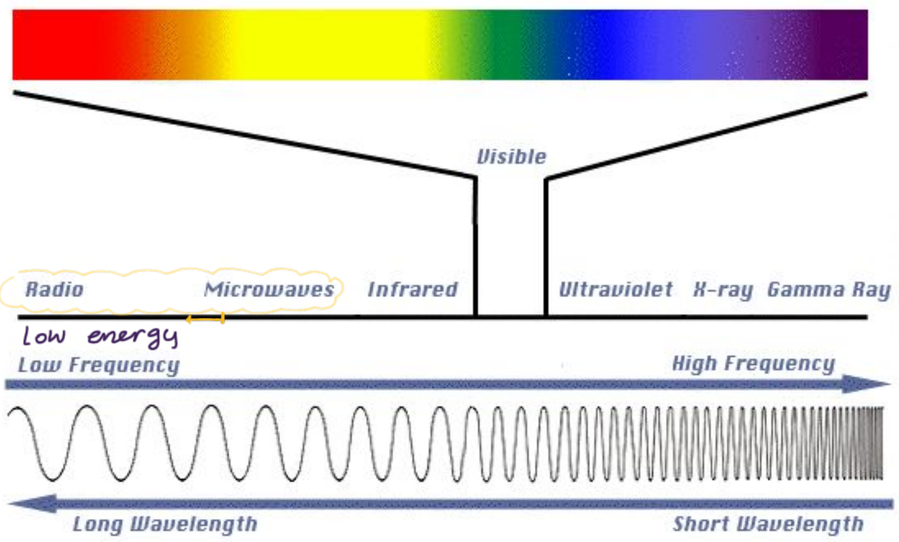
of hydrocarbon compounds

atomic spectroscopy
↓
Flame
qualitative quantitative

IR
vibrational transitions
↓
qualitative only

NMR Spectroscopy

NMR spectroscopy is a form of ***absorption*** spectrometry.



even
↓
equal distribution of charges
↓
ball spherical shape
↓
لاتولد مجال مغناطيسي عند الدوران
↓
NMR inactive

odd
unequal distribution of +ve charge in nucleus
↓
distortion (تشكل النواة غير منتظم)
↓
يولد مجال مغناطيسي عند دوران النواة حول محورها (Nuclear spin)
↓
NMR active

nuclei
even — NMR inactive
odd — NMR Active

NMR تهتم باستجابة النواة

Most absorption techniques (*e.g.* – Ultraviolet-Visible and Infrared) involve the electrons… in the case of NMR, it is the ***nucleus*** of the atom which determines the response.

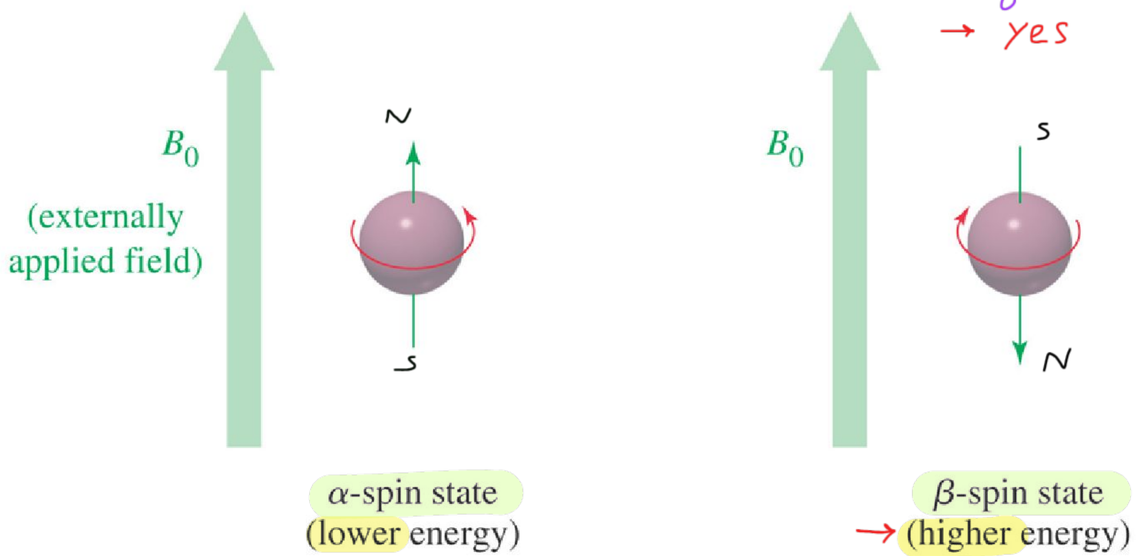
An applied (***magnetic***) field is necessary for the absorption to occur.

of micro - Radio waves

Nuclear Magnetic Resonance (NMR) Spectroscopy

direct observation of the H's and C's of a molecules

Nuclei are positively charged and spin on an axis; they create a tiny magnetic field



Not all nuclei are suitable for NMR.

⇒ ^{1}H and ^{13}C are the most important NMR active nuclei in organic chemistry

Natural Abundance

^{1}H 99.9%

^{13}C 1.1%

^{12}C 98.9% (not NMR active)

$^{2}_{1}H$ (deuterium)

$(^{2}H)_2 \rightarrow D_2O$ مياه ثقيلة

synthetic مصنع

even

كتلة الذرة هي تواتيقيا (تجمع الـ e^- مهملة)

$p^+ + N$

$^{12}_{6}C \rightarrow$ atomic mass / mass number

$^{6} \rightarrow$ atomic number

NMR inactive ✗

عدد p^+ = عدد e^-

عدد N = atomic mass − atomic number

$12 - 6 = 6$

isotopes differ in number of N

isotope

$^{13}_{6}C \rightarrow$ mass number

NMR active ✓

$= 6\,p^+ + 7\,N = 13$

N	e^-	p^+
متغير	ثابت	ثابت

$N = 0$

$^{1}_{1}H \rightarrow$ mass number = كتلة بتواة → only one p^+

NMR active ✓ $^{1}_{1}H \rightarrow$ atomic number = $e^- = p^+$ = one

isotope

$^{2}_{1}H \rightarrow$ mass number = $1\,p^+ + 1N = 2$

NMR active ✓ $^{1}_{1}H \rightarrow$ atomic number

even p^+
even N
= even mass · N
NMR inactive

Spectral Properties, Application and Interactions of Electromagnetic Radiation

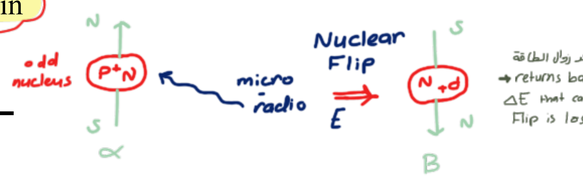
Energy		Wave Number V	Wavelength λ	Frequency υ	Type Radiation	Type spectroscopy	Type Quantum Transition
Kcal/mol	Electron volts, eV	cm^{-1}	cm	Hz			
$x\ 10^{7}$ 9.4	$x\ 10^{6}$ 4.9	$x\ 10^{10}$ 3.3	$x\ 10^{-11}$ 3	10^{21}	Gamma ray	Gamma ray emission	Nuclear
$x\ 10^{3}$ 9.4	$x\ 10^{2}$ 4.9	$x\ 10^{6}$ 3.3	$x\ 10^{-7}$ 3	10^{17}	X-ray	X-ray absorption, emission	Electronic (inner shell)
$x\ 10^{1}$ 9.4	$x\ 10^{0}$ 4.9	$x\ 10^{4}$ 3.3	$x\ 10^{-5}$ 3	10^{15}	Ultra violet / Visible	UV absorption	Electronic (outer shell)
$x\ 10^{-1}$ 9.4	$x\ 10^{-2}$ 4.9	$x\ 10^{2}$ 3.3	$x\ 10^{-3}$ 3	10^{13}	Infrared	IR absorption	Molecular vibration
$x\ 10^{-3}$ 9.4	$x\ 10^{-4}$ 4.9	$x\ 10^{0}$ 3.3	$x\ 10^{-1}$ 3	10^{11}	Micro-wave	Microwave absorption	Molecular rotation
$x\ 10^{-7}$ 9.4	$x\ 10^{-8}$ 4.9	$x\ 10^{-4}$ 3.3	$x\ 10^{3}$ 3	10^{7}	Radio	Nuclear magnetic resonance	Magnetically induced spin states

نهاية الـ micro والـ Radio

radio

- اجهزة الـ NMR المتوفرة حالياً has E needed to flip only ^{1}H & ^{13}C
- other nuclei like ^{2}H (deuterium) & F or N are NMR active but can't be analyzed with NMR E needed to flip them → not available

سقوط هذه الطاقة على النواة

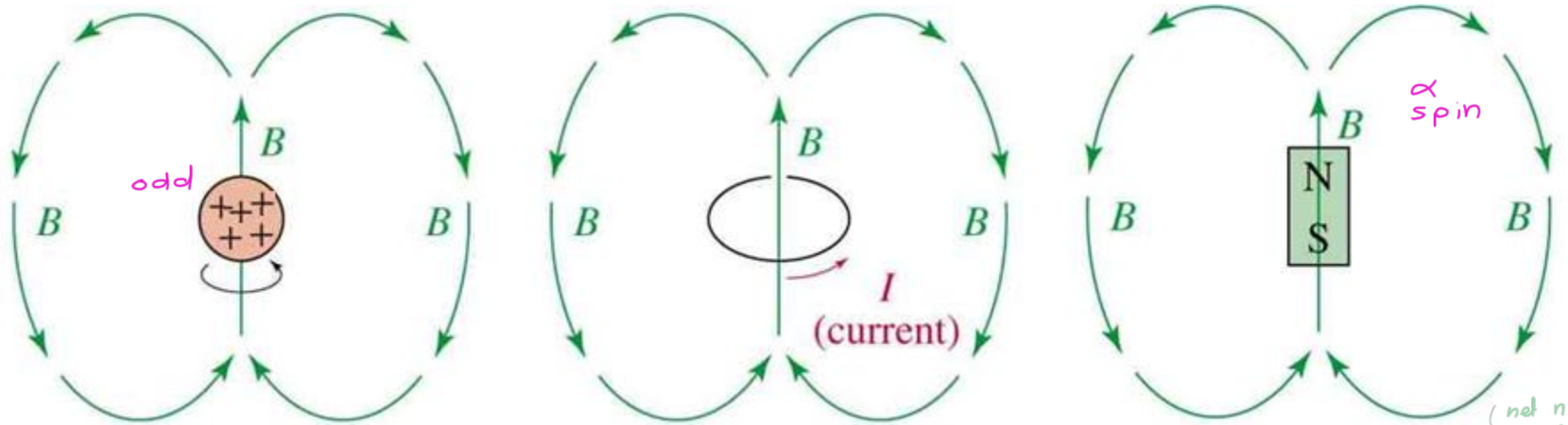


Don't think too literally about the proton physically spinning like a little basketball. In quantum mechanics, "spin" is an intrinsic property of the particle.

Nuclear Spin

عدد p^+ $p^+ + N$

- A nucleus with an odd atomic number or an odd mass number has a nuclear spin.
- The spinning charged nucleus generates a magnetic field.



$^{13}_{6}C$ → 13 - 6 = 7 N odd → 6 p^+ even → half integer spin

$^{14}_{7}N$ → 14 - 7 = 7 N odd → 7 p^+ odd → integer spin

α spin

(nel nucleur spin = 0)

	p^+	N	مجموعهم (mass number)
no spin ←	even 2	+ even 2	= even 4
integer spin (1, 2, 3) ←	odd 3	+ odd 5	= even 8
half integer spin $(\frac{1}{2}, \frac{3}{2}, \frac{5}{2})$ ←	even 4	+ odd 3	= odd 7

اعشار (او العكس)

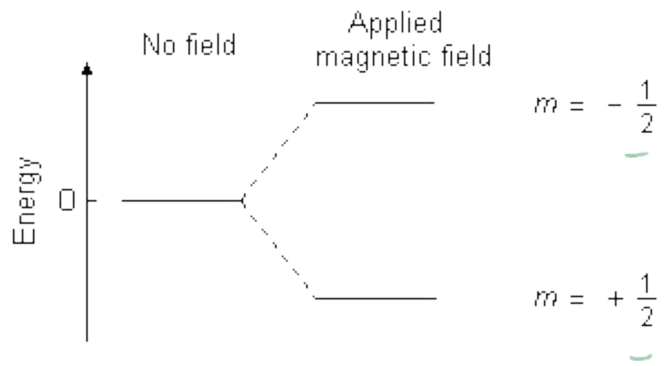
Spin Quantum Numbers

number of possible energy states
For a spin I in a magnatic Feild
determined by Formula 2I +1

The number of spin states is 2I + 1, where I is the spin quantum number.

spin states

Energy levels for a nucleus with spin quantum number 1/2



half integer spin → N & P+ (one even & one odd)

- If the number of neutrons **and** the number of protons are both even, then the nucleus has **NO** spin. (NMR inactive)
- If the number of neutrons **plus** the number of protons is odd, then the nucleus has a half-integer spin (i.e. 1/2, 3/2, 5/2)
- If the number of neutrons **and** the number of protons are both odd, then the nucleus has an integer spin (i.e. 1, 2, 3)

SPIN QUANTUM NUMBERS OF SOME COMMON NUCLEI

التحليل بالـ NMR
only ^{13}C ^{1}H

→ ^{12}C X
inactive

→ ^{2}H
deuterium
E does it match
needed to Flip
E available in device

Most abundant isotopes of C & O don't have spin
(even) (even)

element	^{1}H	^{2}H	^{12}C	^{13}C	^{14}N	^{16}O	^{19}F
NMR active	✓	✓	X	✓	✓	X	✓
	P=1 N=0	P=1 N=1	P=6 N=6	P=6 N=7	P=7 N=7	P=8 N=8	P=9 N=10
Nuclear spin Quantum No. I	$\frac{1}{2}$	1	0	$\frac{1}{2}$	1	0	$\frac{1}{2}$
No. of spin states	2	3	0	2	3	0	2

^{1}H : $2I + 1$
$2(\frac{1}{2}) + 1$
$= 2$

^{14}N : $2I + 1$
$2(1) + 1$
$= 3$

No. p+ لما
or
No. N
or
مجموعهم
⇓
odd

Elements with either odd number of protons or neutrons (odd mass number or odd atomic number) have the property of nuclear "spin". خاصية

p+ N

رياضياً ممكن تساوي صفر
$2(0) + 1 = 1$
لكن ← هذا لا يأخذ بعين الاعتبار لأنها تعتبر
→ has no spin
(even)

The number of spin states is $2I + 1$, where I is the spin quantum number.

odd mass → active

isotope

$^{13}_{6}C$ $P = 6$ $N = 7$ active ✓

$^{12}_{6}C$ $P = 6$ $N = 6$ inactive ✗

^{1}H $P^+ = 1$ $N = 0$ NMR active

مجموع $N + P^+$

Table. General rules for determination of nuclear spin quantum numbers

Mass Number	Number of Protons	Number of Neutrons	Spin (I)	Example
Even	Even 8	Even 8	0	^{16}O
	Odd	Odd	Integer (1,2,...)	^{2}H
	Even	Odd	Half-Integer (1/2, 3/2,...)	^{13}C
Odd	Odd	Even	Half-Integer (1/2, 3/2,...)	^{15}N

NMR inactive ✗

NMR active

NMR active

NMR active

^{2}H $P^+ = 1$ $N = 1$ NMR active

$P^+ = 7$ odd

$N = 15 - 7 = 8$ even

→ half integer

Atoms active in NMR

half Integer
one even one odd

I = 1/2: ^{1}H, ^{13}C, ^{19}F, ^{31}P

Integer

I = 1: ^{2}H, ^{14}N

I = 3/2: ^{15}N

Atoms not active in NMR

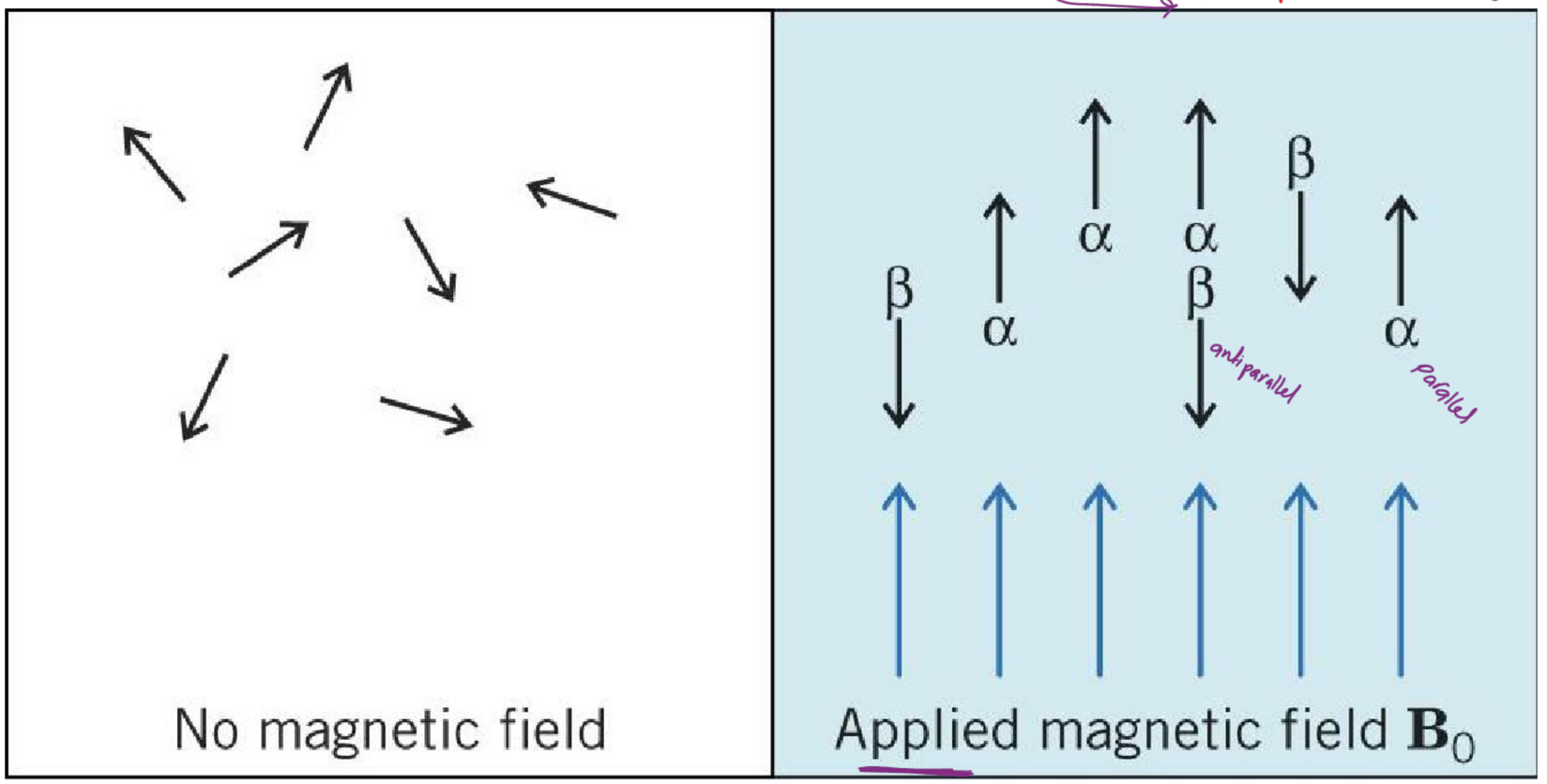
I= 0: ^{12}C, ^{16}O

odd nuclei (already have a magnitic Feild)

B_0 → parallel α

Anti parallel β higher energy

الذرات
Freely تتحرك
وبكل الاتجاهات
حركة عشوائية

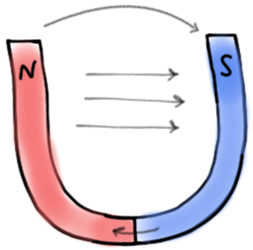


aligned nuclei

restricts their movement

(a)

by NMR جهاز (b)

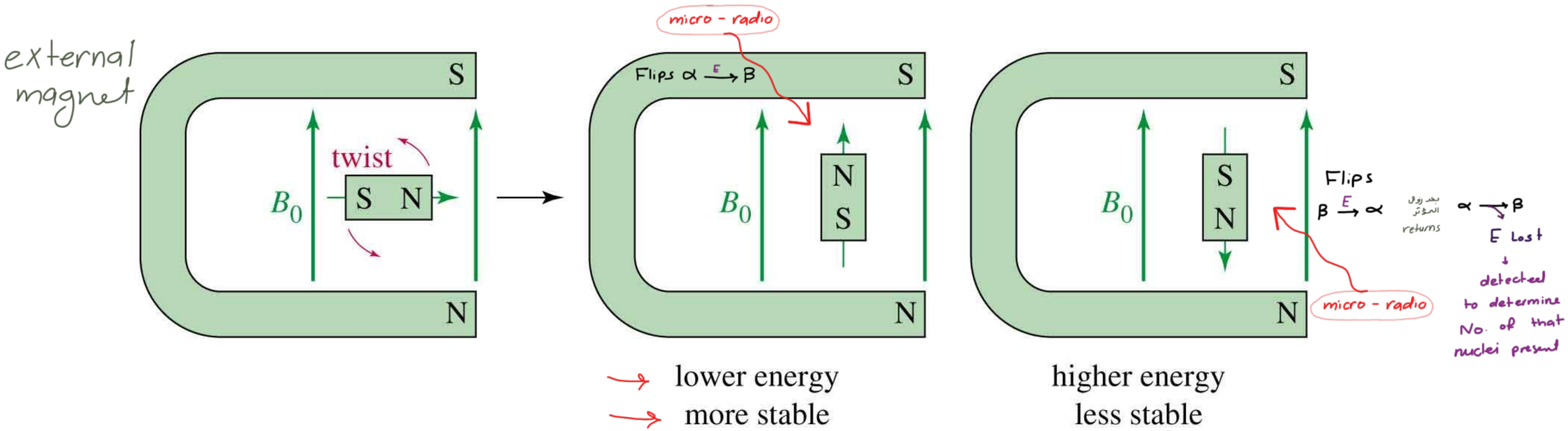


اتجاه المجال المغناطيسي

inside magnet : S ⟶ N

outside : N ⟶ S

Behavior of spinning protons with external magnetic field



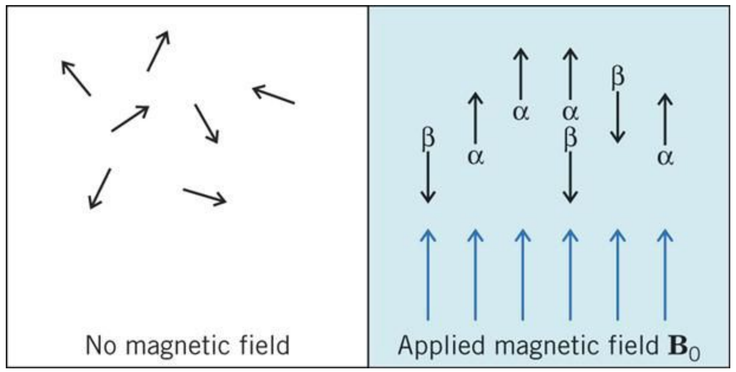
(α-spin state)

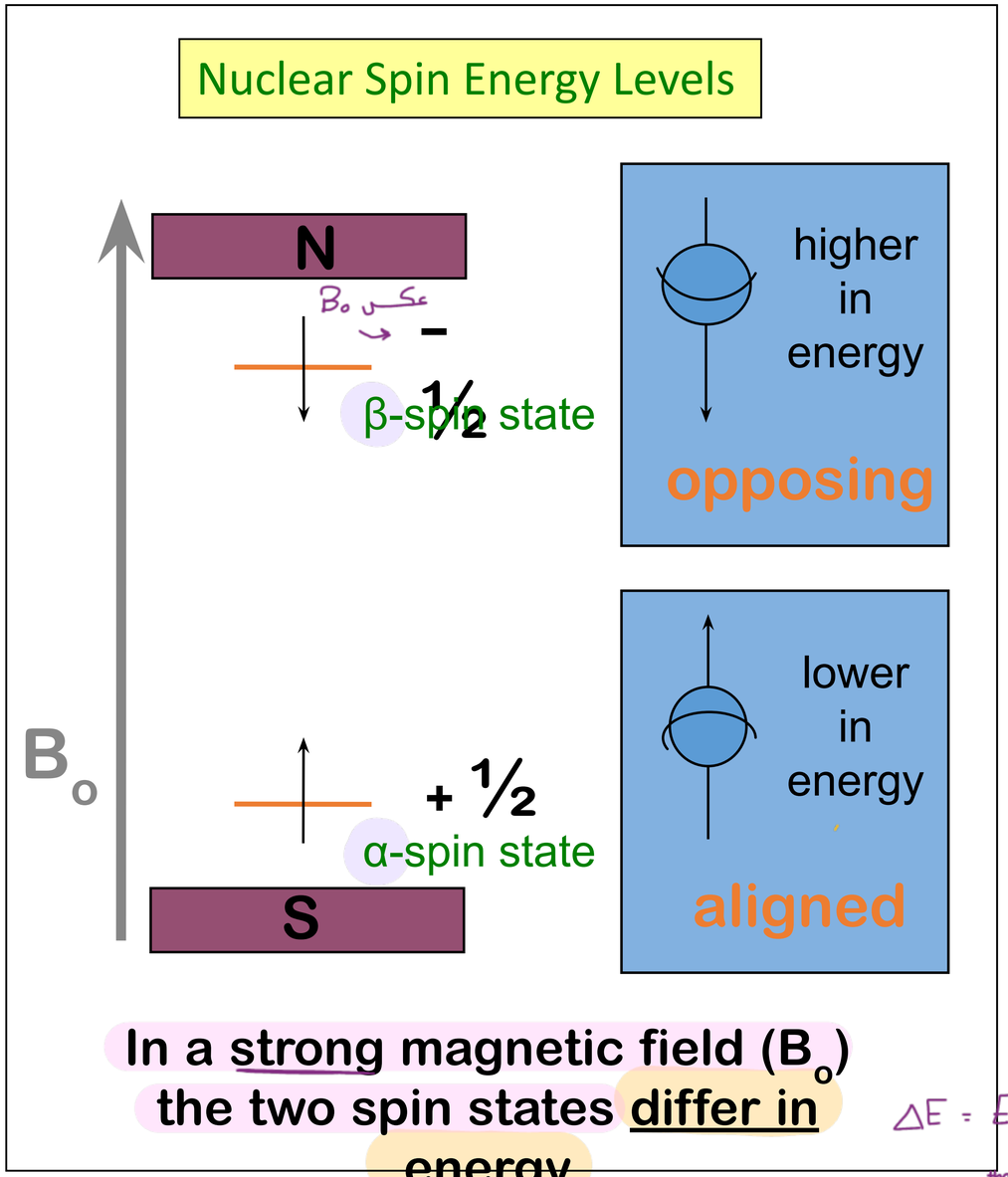
اتجاه external magnetic Feild B_0 = اتجاه magnetic Feild of nuclei

(β-spin state)

THE NUCLEUS IN A MAGNETIC FIELD

When nuclei are exposed to external magnetic field of strength B_0, their spins line up parallel to the applied field, either spin aligned (α-spin state) or spin opposed (β-spin state) to the external field.





Without an external magnetic field:

The two spin orientations have essentially the same energy.

$\Delta E = E$

micro radio that causes the Flip

ΔE and Magnet Strength

The energy difference between aligned (α) and opposed (β) to the external magnetic field (Bo) is generally small and is

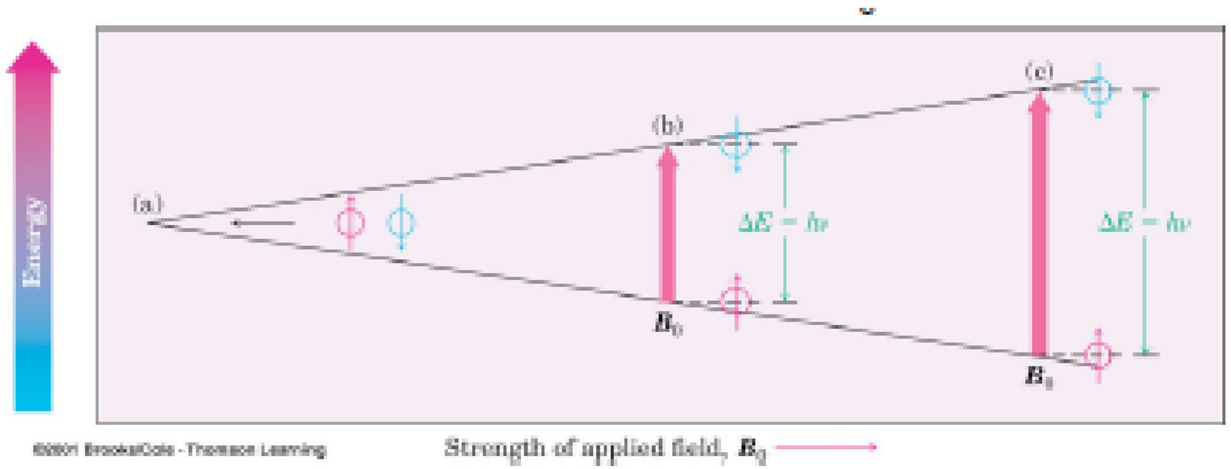
⇒ dependent upon Bo

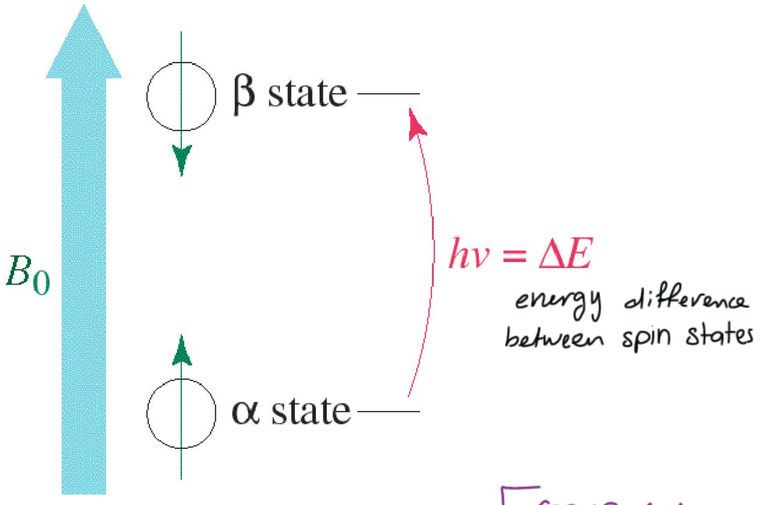
micro الى نهاية ارتفاع

Applied EM radiation (radio waves) causes the spin to flip and the nuclei are said to be in ***resonance*** with Bo

↑ Bo magnet strength

↑ ΔE energy needed to Flip ($E_\beta - E_\alpha$)





γ tells us how strongly a particular nucleus interacts with a magnetic field

So different nuclei behave differently in the same magnetic field.

That's why ^1H and ^{13}C don't resonate at exactly the same frequency.

$$\Delta E = h\nu \qquad \Delta E = h\frac{\gamma}{2\pi}B_0 \qquad \nu = \frac{\gamma}{2\pi}B_0$$

(s^{-1} or Hz)

B_o = external magnetic field strength (gauss)

γ = gyromagnetic ratio (characteristic for each nuclei)

- $^1H = 26{,}752\ s^{-1}gauss^{-1}$
- $^{13}C = 6.7\ s^{-1}gauss^{-1}$

Frequency

$\nu = \frac{\gamma}{2\pi} B_o$ ← تتعين دائرة

$B_o = 14.092$ gauss

$= \frac{26.752}{2\pi} \times 14.092$

$\nu_{H^1} = 60$ MHz

$\nu = \frac{\gamma B_o}{2\pi} = \frac{6.7 \times 14.092}{2\pi}$

$\nu_{C^{13}} = 15.02$ MHz

Bo

. In a 14,092 gauss field, a 60 MHz (60,000,000) photon is required to flip a proton.

photon's $\nu < 60$ MHz

→ ^1H nuclei won't Flip

ν used in NMR : **. Low energy, radio frequency.**

ΔE and Magnet Strength

The energy difference between aligned and opposed to the external magnetic field (Bo) is generally small and is dependent upon Bo

Applied EM radiation (radio waves) causes the spin to flip and the nuclei are said to be in ***resonance*** with Bo

$\Delta E\ {}^{1}H > \Delta E\ {}^{13}C$

due to صغر حجم ^{1}H

تجاذب انويته عالي ↑ α ↓ β

المسافة بينهم صغيرة

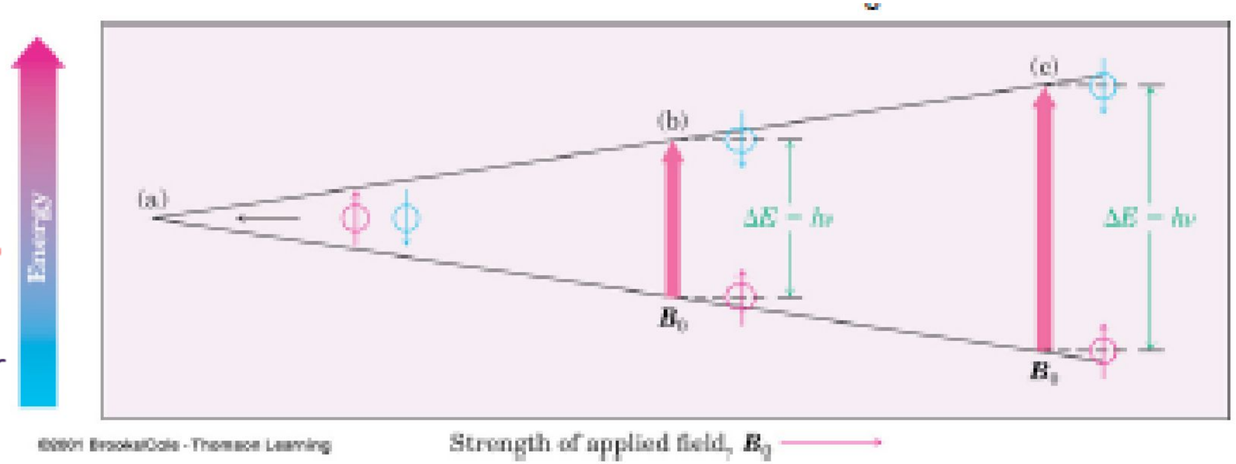
harder to Flip ↑ اذن احتاج

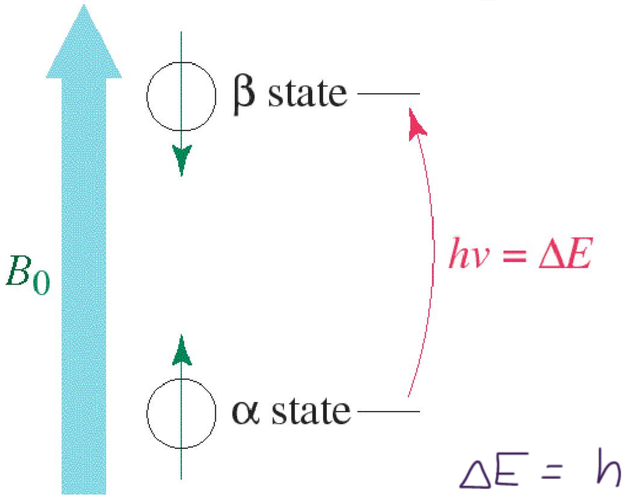
X4

مقارنة بـ E

needed to Flip C easier

→ Larger size





$$\Delta E = h\nu$$

$$\nu = (\gamma / 2\pi)B_o$$

B_o = external magnetic field strength

γ = gyromagnetic ratio

^{1}H = 26752 rad $s^{-1}gauss^{-1}$ = 2.6752 X10^{8} rad $s^{-1}T^{-1}$

^{13}C = 6728284 rad $s^{-1}gauss^{-1}$ = 6.728284 X10^{7} rad $s^{-1}T^{-1}$

$\Delta E = h\nu$

$\nu = \frac{\gamma}{2\pi} B_o$

$= \frac{26752\ rad\ s^{-1}\ gauss^{-1}}{2\pi \times 10^{6}} \times 14092\ gauss$

$= 60\ MHz$

6.6×10^{-27}

. **h= Plank's constant= 6.63x 10^{-27} erg. S**

. **In a 14092 gauss field, a 60 MHz (60,000,000) photon is required to flip a proton.**

. **Low energy, radio frequency.**

The rad is a unit of absorbed radiation dose, defined as 1 rad = 0.01 Gy = 0.01 J/kg

Magnetic Shielding

in nuclei

If all protons absorbed the same amount of energy in a given magnetic field, not much information could be obtained.

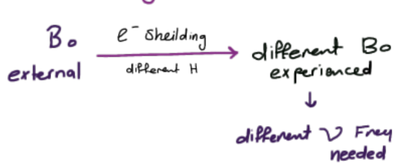
But protons are surrounded by electrons that shield them from the external field.

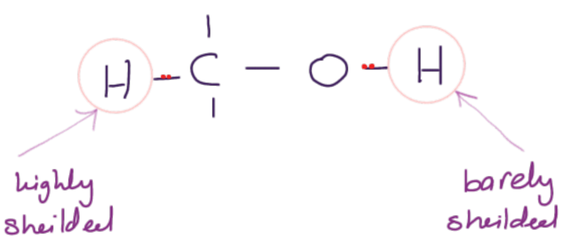
get in the way

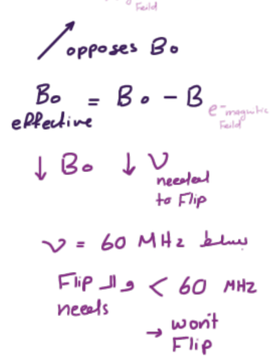
⇒ Circulating electrons create an induced magnetic field that opposes the external magnetic field.

حركة الـ e تولد مجال مغناطيسي
يعاكس Bo يقاومه

كل H رح تمتص E مختلفة لان
e⁻ density differs for each nuclei







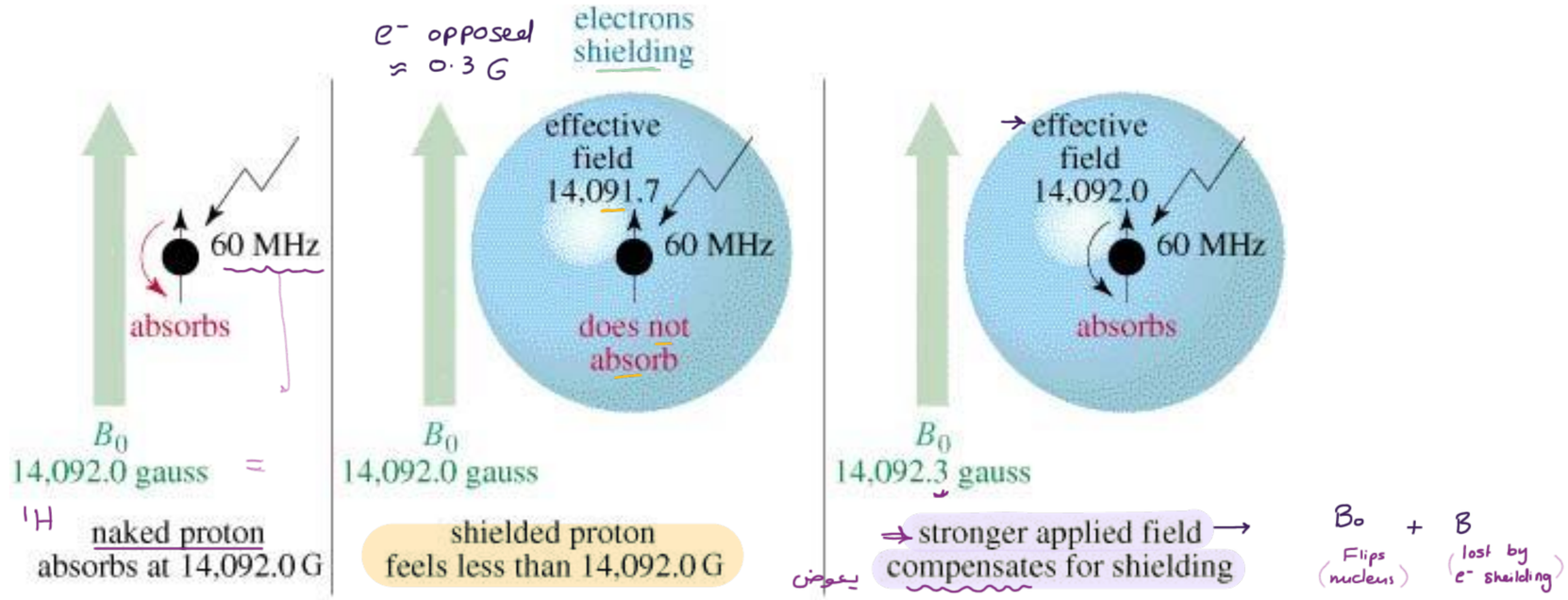
Shielded Protons

B_o

Magnetic field strength must be increased for a shielded proton to flip at the same frequency.

لتعويض تأثير الـ e^-

$B_o \propto \Delta E$
ν

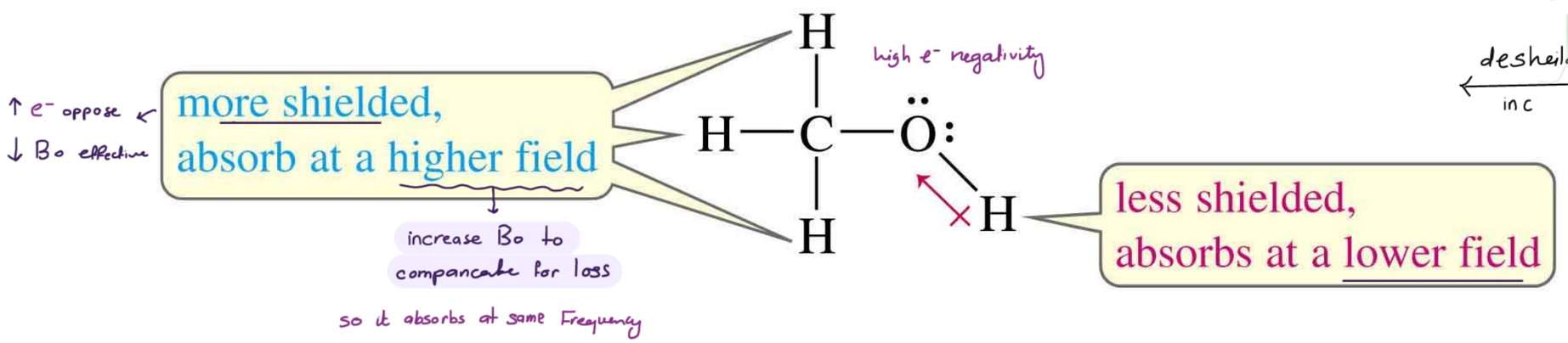


Protons in a Molecule

atoms attached to
e⁻ density around nuclei

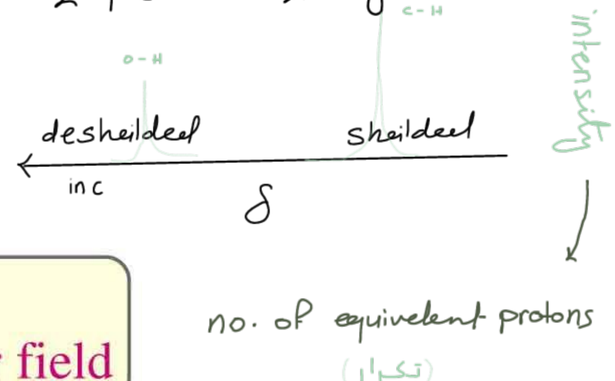
H

Depending on their chemical environment, protons in a molecule are shielded by different amounts.

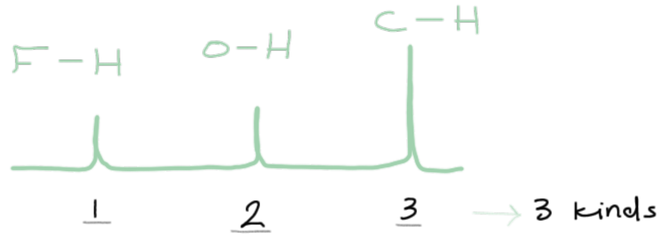


2 proton types < C – H / O – H

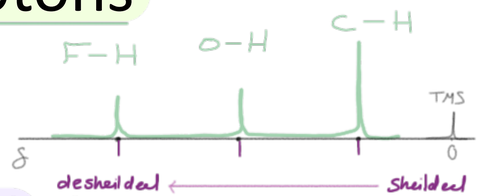
2 peaks – 2 signals



NMR Signals



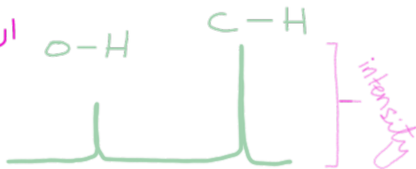
- The ***number*** of signals shows how many different kinds of protons are present.



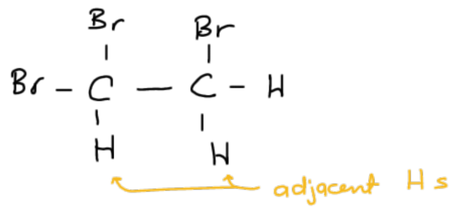
- The ***location*** of the signals shows how shielded or deshielded the proton is.

- The ***intensity*** of the signal shows the number of protons of that type.

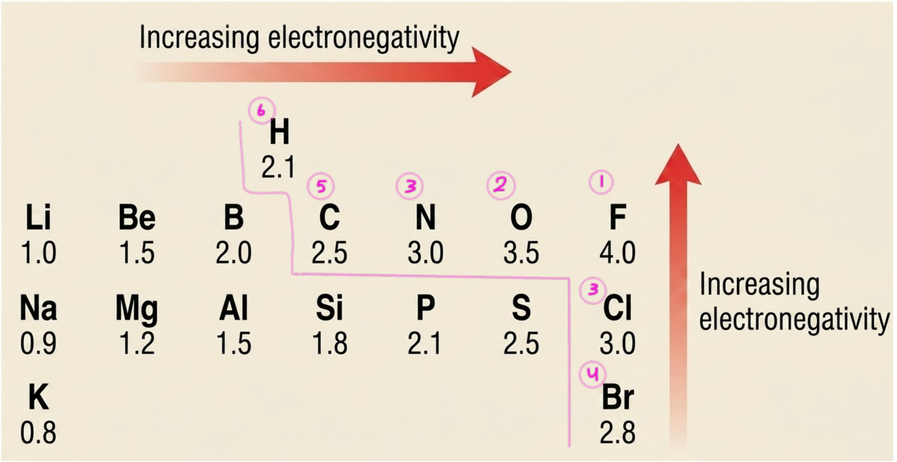
ارتفاع الـ peak يزداد كلما زاد عدد الـ H من نفس النوع

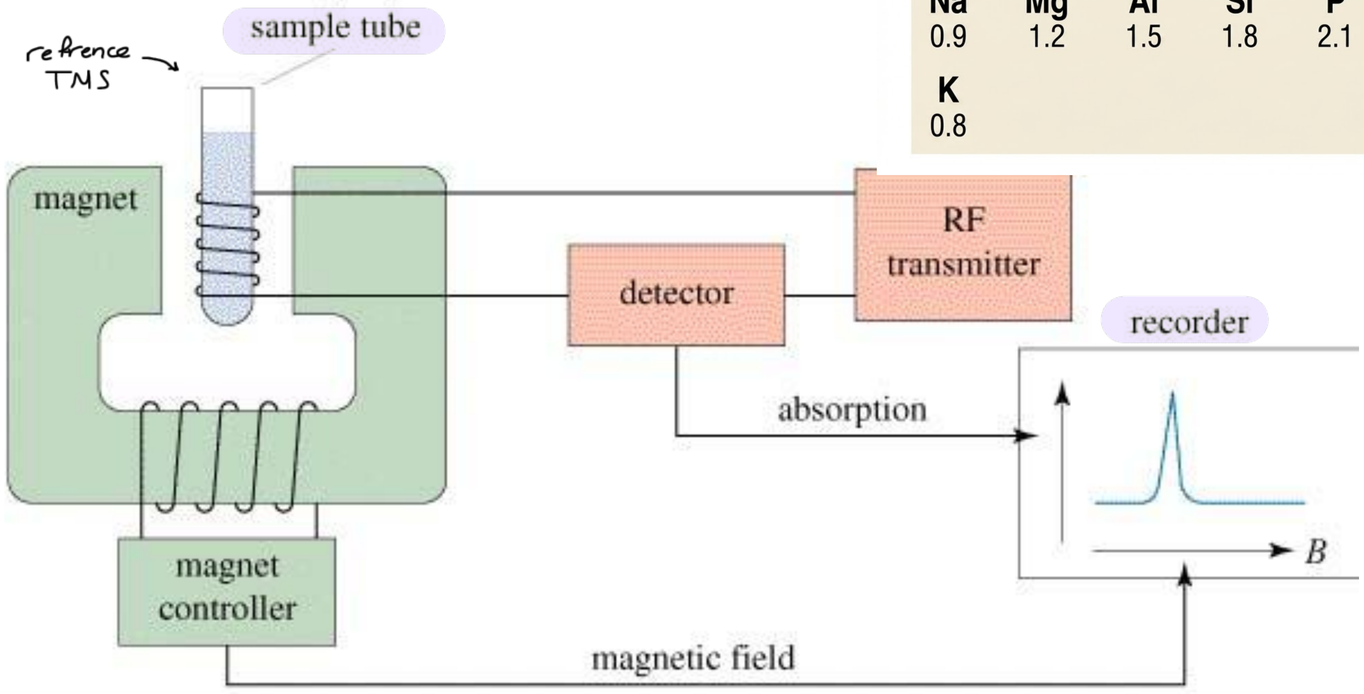


- Signal ***splitting*** shows the number of protons on adjacent atoms.



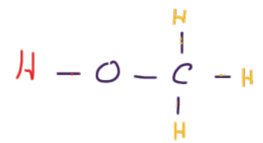
The NMR Spectrometer





The NMR Graph

hydrogens differ



e⁻ sheilding
↓
loss of B_o
↓ B_o effective
→ compansation intensity lost

يضعف المجال المغناطيسي المؤثر على النواة

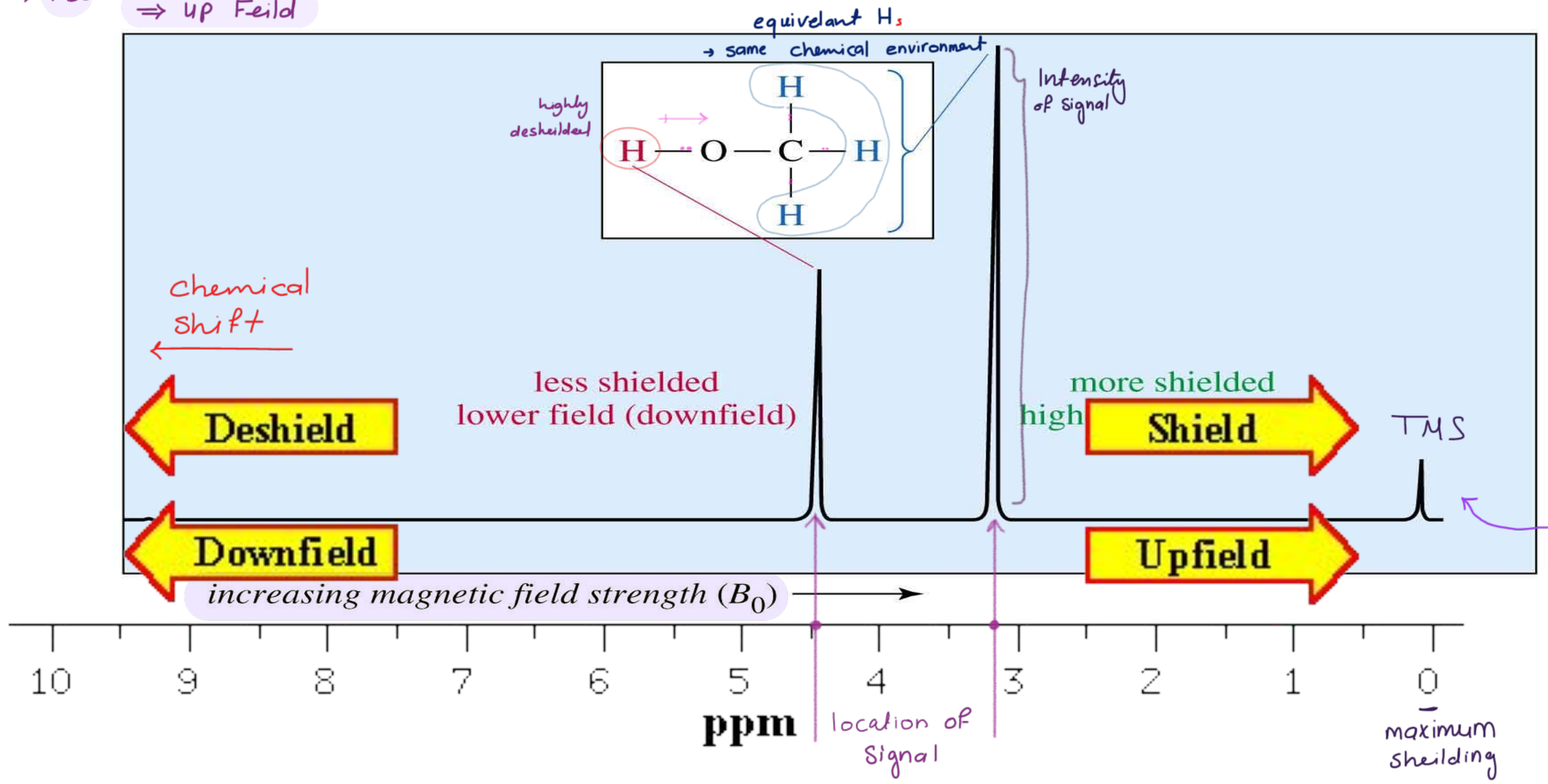
للتعويض عن الخسارة

C : H sheilded → ↑ B_o

O : H desheilded

⇒ up Feild

NMR
- ^1H proton NMR
- ^{13}C NMR



* تساؤل شخصي !
مع رد الدكتور

ليش الـ Peak معجزة وهي لـ 12 H !!

لـ $Si-CH_3$ ←
3 equivelent H → Peak ارتفاعها 3 H

TMS → 4 X $-CH_3$
↓
لكل وحدة ارتفاعها ← 3 H
زي بعض بالزبط → و الـ CH_3 ربع

Signal الـ → Peak ارتفاعها 3H تكررت مرات ٤ هزوه بعض (مايجمعو)

e⁻ pair in middle
very close in electronegativity

H : C

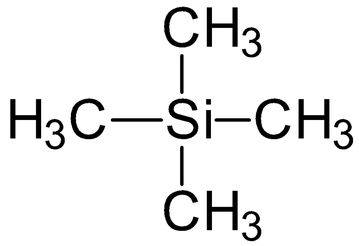
Pure covalent bond

↓

Sheildeel

sample
- solvent
- my compound
- TMS

Tetramethylsilane



- TMS is added to the sample. → refrence compound
- Since silicon is less electronegative than carbon, TMS protons are highly shielded. Signal defined as zero.

Si — C

maximum sheilding of H

- Organic protons absorb downfield (to the left) of the TMS signal.

C – H

δ = 0 ppm

اي مركب كان بالعينة لازم يجي بعده spectrum عن الـ refrence هو TMS

0 / TMS البعد عن

desheilded ← sheilded

Chemical Shift

ppm

- Measured in parts per million.
- Ratio of shift downfield (left) from TMS (Hz) to total spectrometer frequency (Hz).
- Same value for 60, 100, or 300 MHz machine.
- Called the **delta scale (δ)**.

↑ B_o ↑ ν or E needed to Flip

Chemical Shift calculation

Hz zero MHz

$$\delta = V_H - V_{TMS} / V_{NMR} \times 10^6 \text{ ppm}$$

(Hz) (zero)

$$\delta = \frac{\nu_H - \nu_{TMS}}{\nu_{NMR} \times 10^6}$$

(MHz)

= ..... ppm

δ= Chemical shift (ppm)

V_H= Frequency of proton

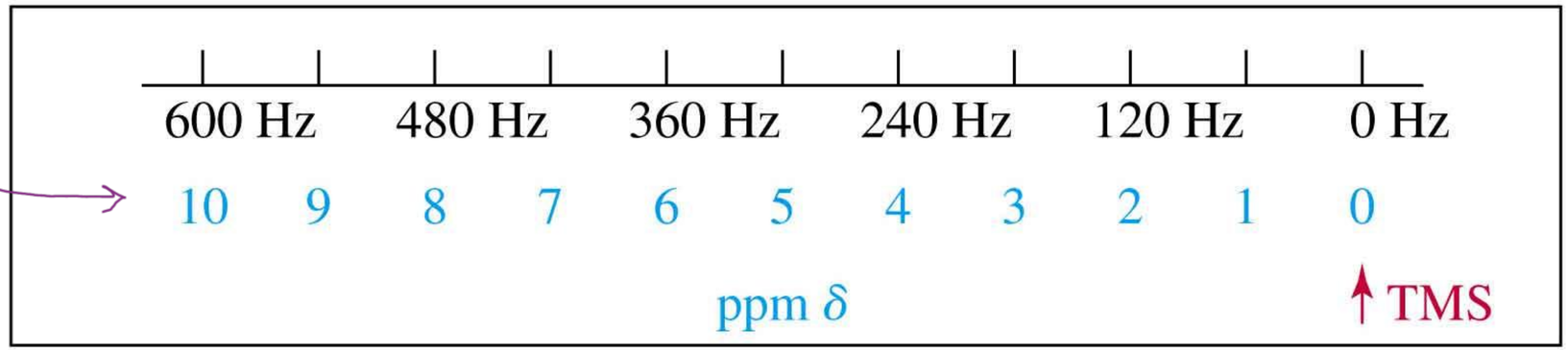
V_{TMS}= 0

V_{NMR}= 60 MHz or 100MHZ or 300 MHz

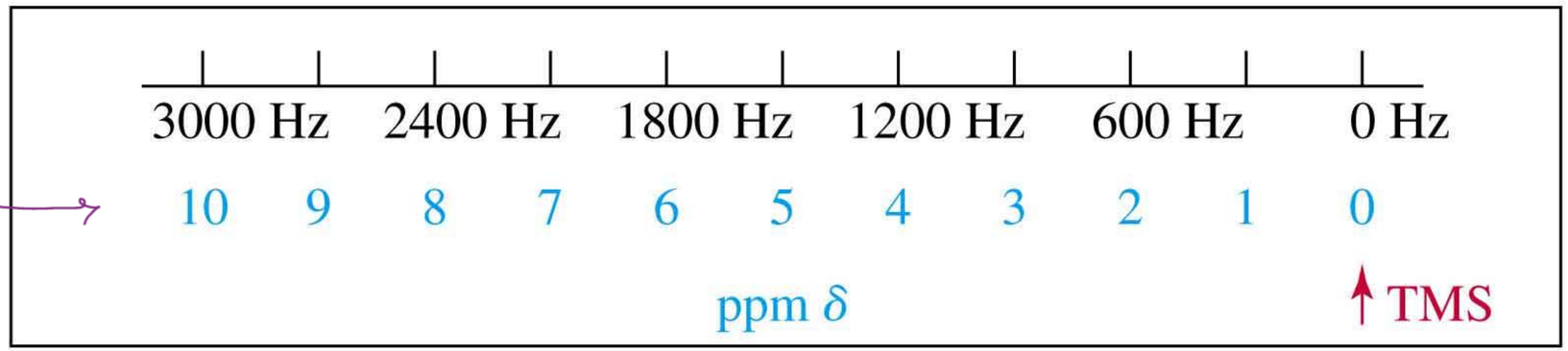
$1MHz = 10^6$ Hz

Delta Scale

$$\text{chemical shift, ppm } \delta = \frac{\text{shift downfield from TMS (in Hz)}}{\text{spectrometer frequency (in MHz)}}$$

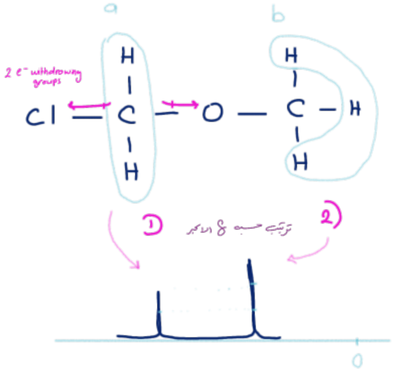


60 MHz



300 MHz

300 Hz / 90 MHz



Example: Cl-CH2-O-CH3 shows 2 absorptions for H NMR and two for C NMR on a 90 MHz NMR, H resonances are at 300 Hz and 480 Hz (the instrument is tuned so that TMS absorbs at exactly 90 MHz) calculate the δ delta for both proton and carbon.

For H NMR

δ = 300 Hz - 0 / 90 MHz x 106 = 3.3 ppm = 3.3×10^{-6}

δ = 480 Hz - 0 / 90 MHz x 106 = 5.3 ppm

for C NMR, the absorptions are at 1290 Hz and 1910 Hz (where TMS is at 22,6 MHz)

δ = 1290 Hz- 0 / 22.6 MHz x 106 = 57.1 ppm

δ = 1910 Hz- 0 / 22.6 MHz x 106 = 84.5 ppm

TABLE 13-2 Chemical Shifts of the Chloromethanes

Compound	Chemical Shift	Difference
methane		
CH_4	δ0.2	
		2.8 ppm
CH_3Cl	δ3.0	
		2.3 ppm
CH_2Cl_2	δ5.3	
		1.9 ppm
$CHCl_3$	δ7.2	

highly sheilded

e⁻ withdrowing

Note: Each chlorine atom added changes the chemical shift of the remaining methyl protons by about 2 to 3 ppm. These changes are nearly additive.

Location of Signals

e⁻ Farther From H nucleus

- More electronegative atoms deshield more and give larger shift values. δ

e⁻ withdrowing group

كلما بعدت الـ e⁻ withdrowing group عن الـ H ↓ قل سحبها

e⁻ withdrowing

- Effect decreases with distance.

- Additional electronegative atoms cause increase in chemical shift. δ

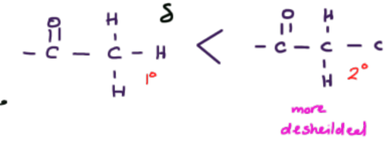
↑ desheildeel

↑ e⁻ withdrowing groups ↓ sheilding ↑ chemical shift δ

اشياء احنها بعين الاعتبار عند مقارنة H لتحديد δ

- No. of e⁻ withdrowing groups effecting H
- attachement of H to withdrowing group directly attached > near > Far
- number of H the group withdrowing From

carbonyl سحب الـ
3 H موزع على
→ less effective
2 H من السحب في



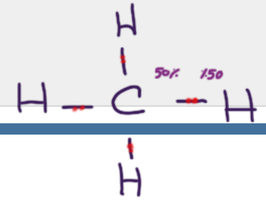
↑ electronegativity difference F : H
↑ desheilding
↑ δ delta
(to the left / Farther from TMS)

F → 1st most electronegative atom
O → 2nd " "

3 e⁻ withdrowing groups

O more electronegative than Cl

$CHCl_3$	CH_2Cl_2	CH_3F	CH_3OH	CH_3Cl	CH_3Br	CH_3I	CH_4	$(CH_3)_4Si$
7.27	5.30	4.26	3.4	3.05	2.68	2.16	0.23	0



the highest sheildeed δ = 0

highly sheildeed

e⁻ الكربون بجذب barely
e⁻ negativity حزمه الـ
بينه وبين الـ H قليله

e⁻ negativity
C > Si

Si
لسا سحبه اقل
e⁻ negativity وحزمه الـ
اقل

↑ e⁻ negativity
↑ delta δ

$CH_3F > CH_3OH > CH_3Cl > CH_3Br > CH_3I$

↑δ → ↓δ
arrange in decreasing chemical shift
CH_3OH, CH_3F, CH_2Cl_2, CH_3Cl

$CH_2Cl_2 > CH_3F > CH_3OH > CH_3Cl$

Typical Values

$H^{1°}$ → H attached to a C that is attached to H_3 or one R (one C)

$H^{2°}$ → H attached to a C that is attached to 2C or 2R

$H^{3°}$ → H attached to a C that is attached to 3C or 3R

δ inc

ترتيب وقوع الإشارة δ

carboxylic A $R-\overset{O}{\overset{\|}{C}}-OH$ (1)

indirect $R-\overset{O}{\overset{\|}{C}}-CH_3$ (3)

direct $R-\overset{O}{\overset{\|}{C}}-H$ (2)

Type of Proton	Approximate δ
alkane ($-CH_3$) 1°	0.9
alkane ($-CH_2-$) 2°	1.3
alkane ($-\underset{|}{CH}-$) 3°	1.4
ketone / carbonyl $-\overset{O}{\overset{\|}{C}}-CH_3$ (2 e⁻ withdrawing units)	2.1
triple bond $-C\equiv C-H$ (direct)	2.5
$R-CH_2-X$ (X = halogen, O)	3–4
Alkene $>C=C<_{H}$ (directly attached)	5–6

Type of Proton	Approximate δ
Alkene $>C=C<_{CH_3}$ (indirectly attached (weaker than direct))	1.7
benzene ring $Ph-H$ (directly attached)	7.2
$Ph-CH_3$ (indirectly)	2.3
$R-CHO$ Aldehyde	9–10
$R-COOH$ carboxylic acid (largest δ)	10–12
Aliphatic $R-OH$	variable, about 2–5
Aromatic $Ar-OH$	variable, about 4–7
$R-NH_2$	variable, about 1.5–4

$-\overset{O}{\overset{\|}{C}}-H$ (direct) > $-\overset{O}{\overset{\|}{C}}-CH_3$

الأكثر سحب (strongest withdrawing) الأقل سحب deshield

CH_3-O-H

2 e⁻ withdrawing groups

δ ≡ < =

$H-C\equiv C-H < H-C=C-H$

سحب e⁻ أقل due to high e⁻ density on C

$CH_3-\ddot{N}(H)-H$ < $CH_3-CH_3-\ddot{N}:$

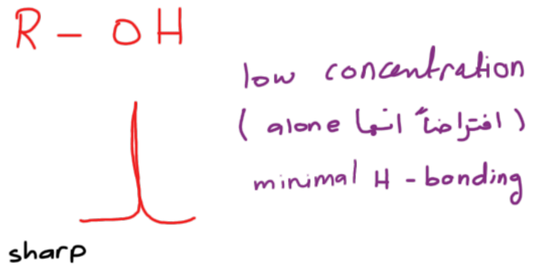
primary amine — 2nd amine

e⁻ donating groups

↑ electronegativity of N

سحب e⁻ ↑

Note: These values are approximate, as all chemical shifts are affected by neighboring substituents. The numbers given here assume that alkyl groups are the only other substituents present. A more complete table of chemical shifts appears in Appendix 1.

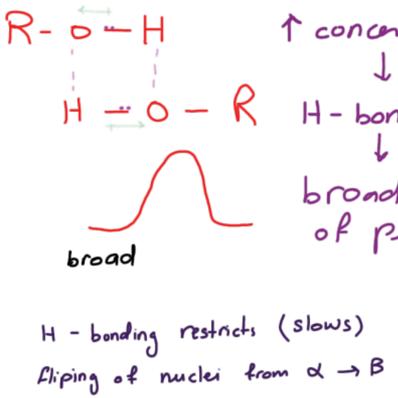


δ ∝ concentration

↑ concentration ↑ physical interactions

↑ deshilding δ + broadness of peak

O-H and N-H Signals



δ

- Chemical shift depends on concentration.

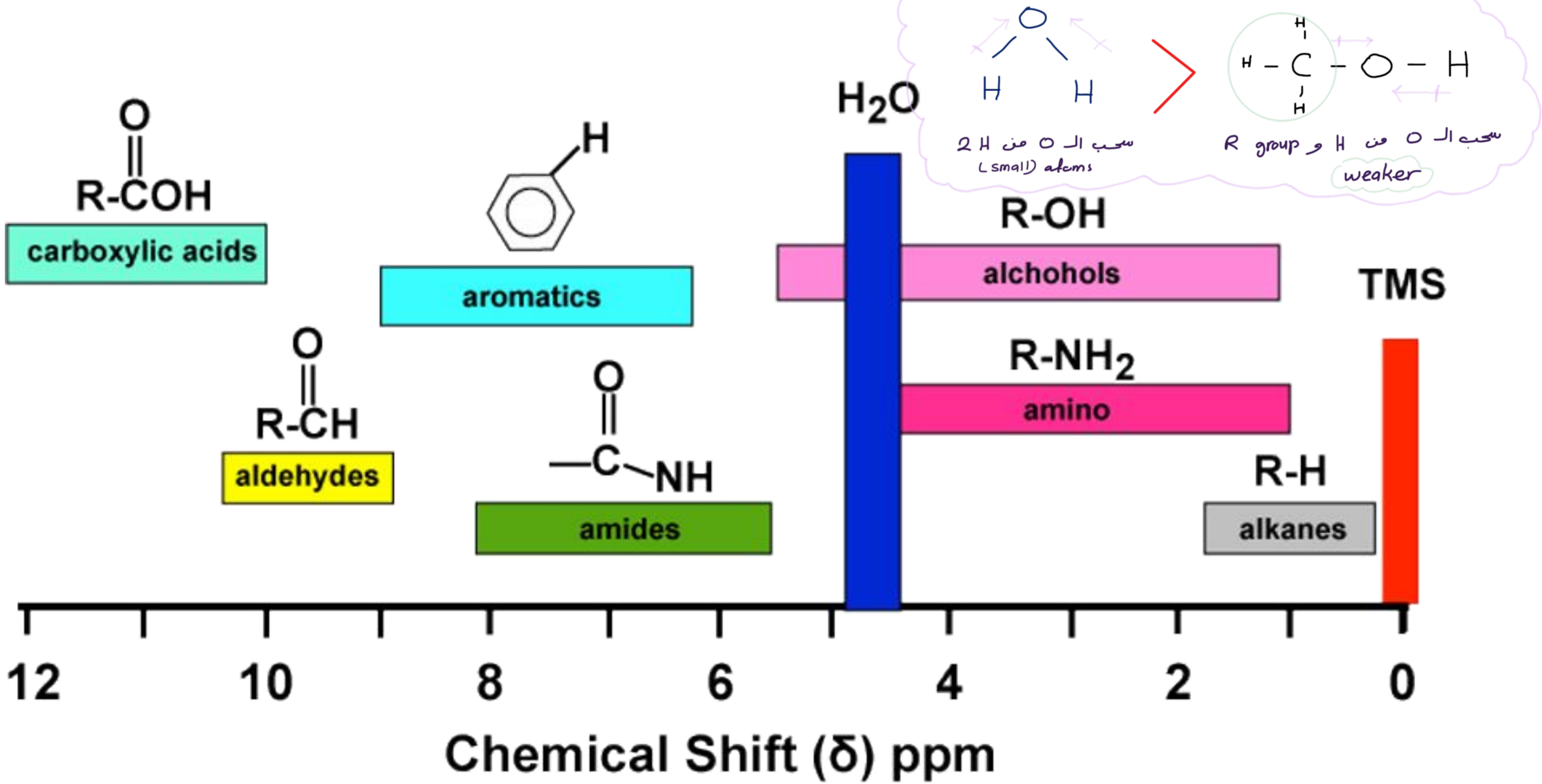
physical interactions

1

- Hydrogen bonding in concentrated solutions deshield the protons, so signal is around δ3.5 for N-H and δ4.5 for O-H.

2

- Proton exchanges between the molecules broaden the peak.


H2O
R-OH
alchohols
TMS
R-NH2
amino
R-H
alkanes
carboxylic acids
aromatics
aldehydes
amides
12
10
8
6
4
2
0
Chemical Shift (δ) ppm
سحب الـ O من 2 H
(small) atoms
سحب الـ O من H و R group
weaker

C N O F
Si P S Cl

maximum
↳ desheilding

Carboxylic Acid Proton, δ10+

* having empirical Formula

$C_2H_4O_2$

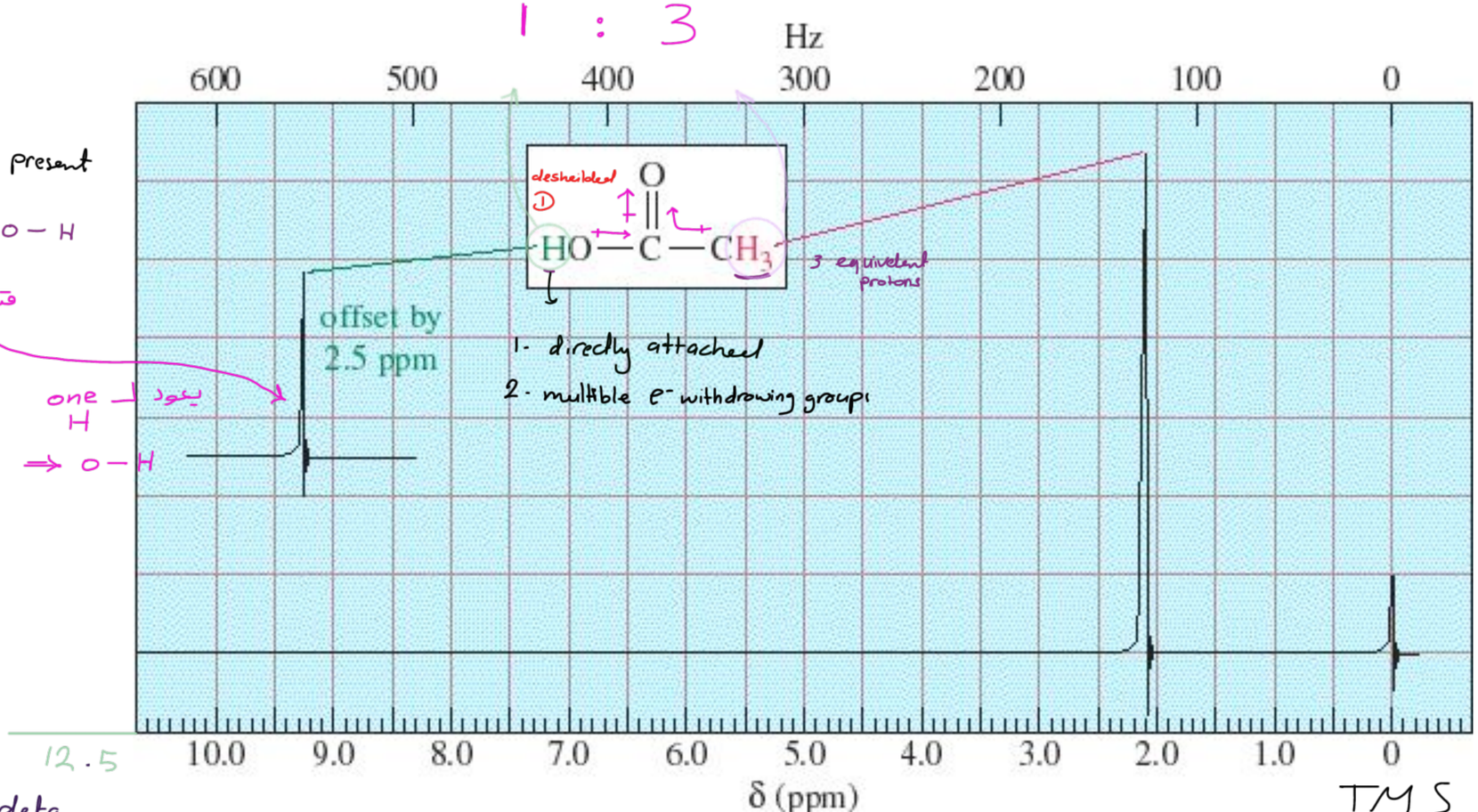
IHD =1

IR analysis
↳ functional groups present

$-\overset{|}{\underset{|}{C}}-H$ $-\overset{O}{\overset{\|}{C}}-$ $-O-H$

قدرت اعرف انه
↓
واحد الـ
Structural Formula

one H يعود ل
⇒ O−H



or deta
Peak at δ

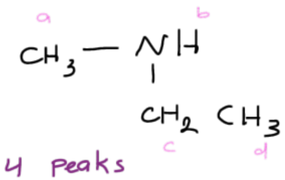
Proton NMR

CH_4
one peak

$CH_3\ CH_3$
one peak

$CH_3\ CH_2\ CH_3$
2 peaks

$CH_3\ CH_2\ CH_2\ CH_3$
2 peaks



4 peaks

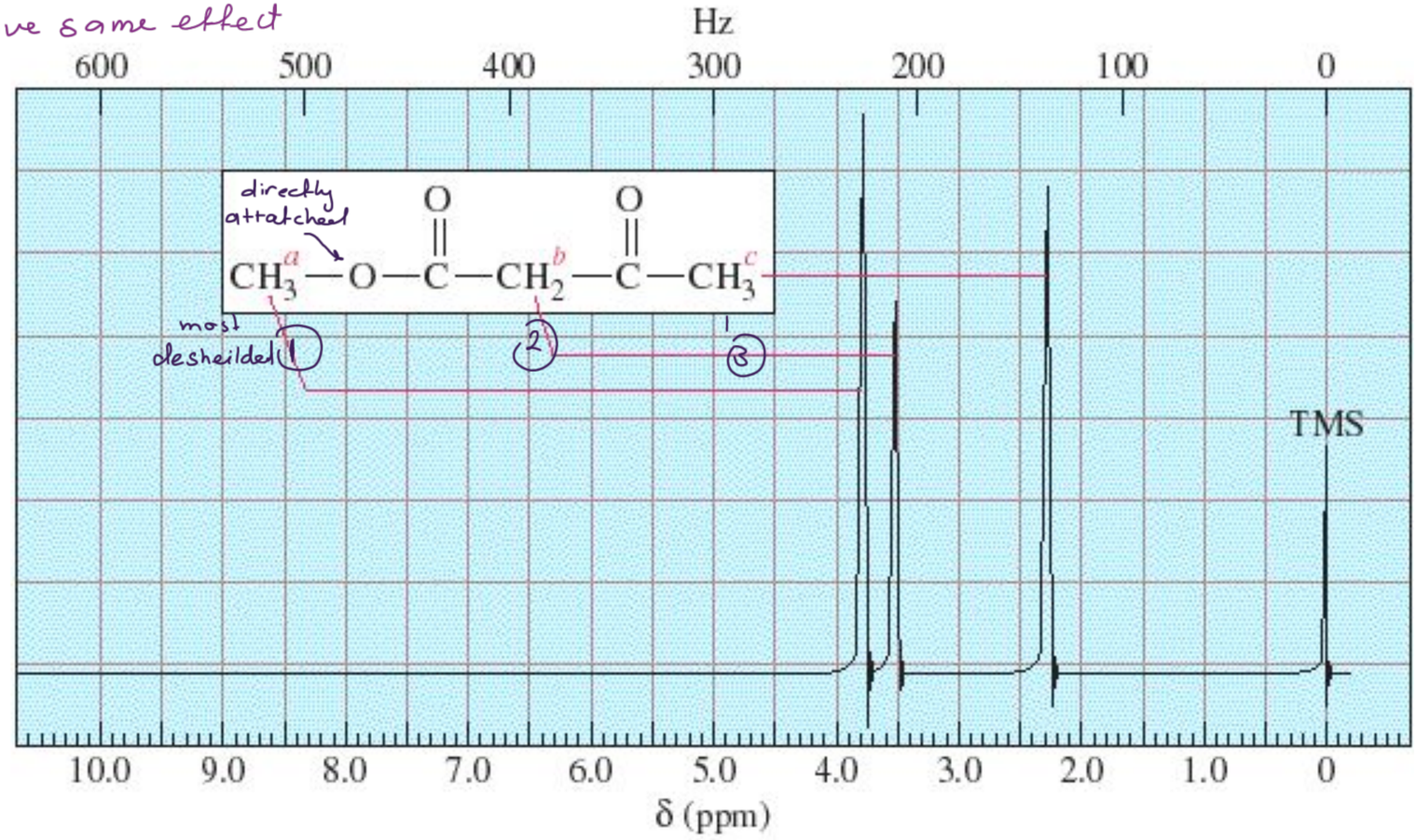
plan of symmetry

one peak

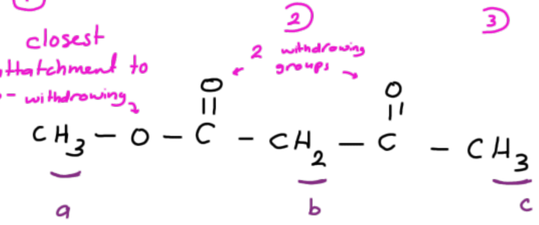
Number of Signals

Equivalent hydrogens have the same chemical shift.

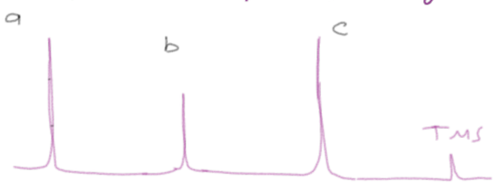
on the same C
& have same effect



deshielded
1 closest attatchment to e⁻ withdrawing
2 2 withdrawing groups
3

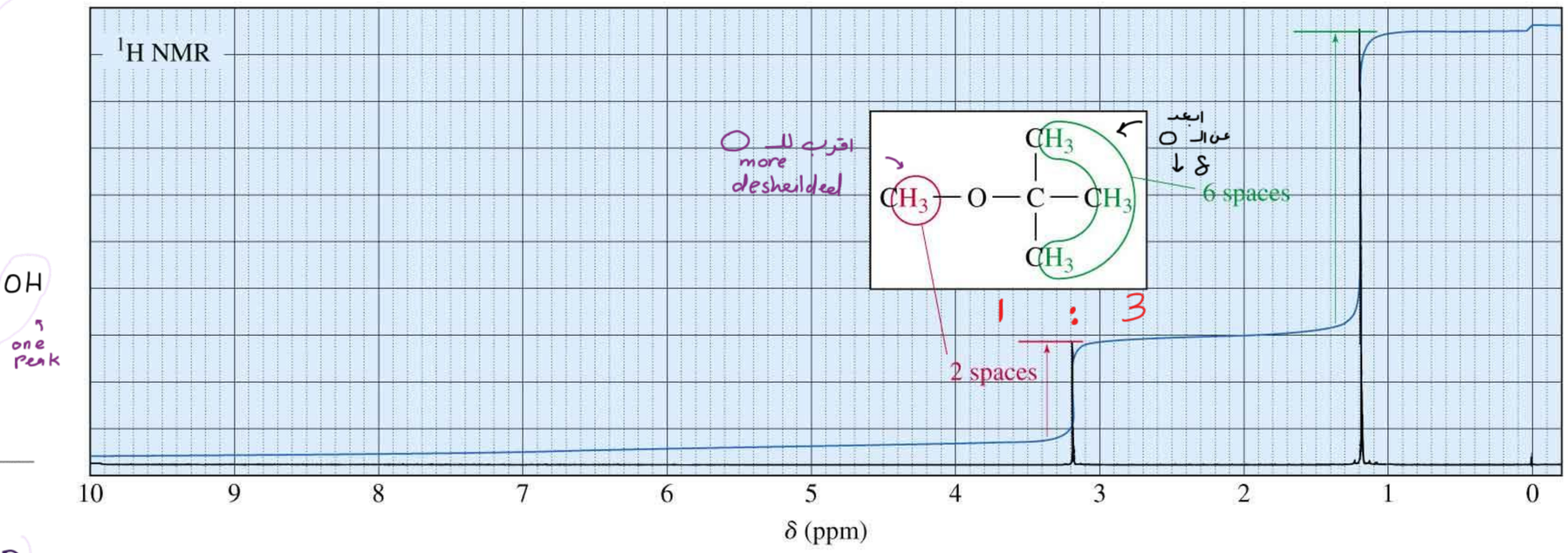


3 H kinds
separated → 3 peaks (no splitting)



Intensity of Signals

- The area under each peak is proportional to the number of protons.
- Shown by integral trace.



How Many Hydrogens?

When the molecular formula is known, each integral rise can be assigned to a particular number of hydrogens.