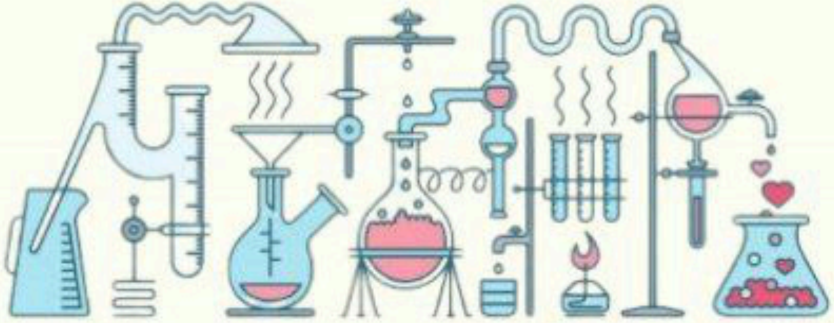
تفريغ تحليل آلي



اسم الموضوع: NMR✨

Part 1

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Soul Academy

لجان الدفعات

Nuclear Magnetic Resonance Spectroscopy

Qualitative
Not destructive

كل الشغل على

$N^{\pm}$
P^{+}

nucleus

nutrons & Proton

$N^{\pm}$ P^{+}

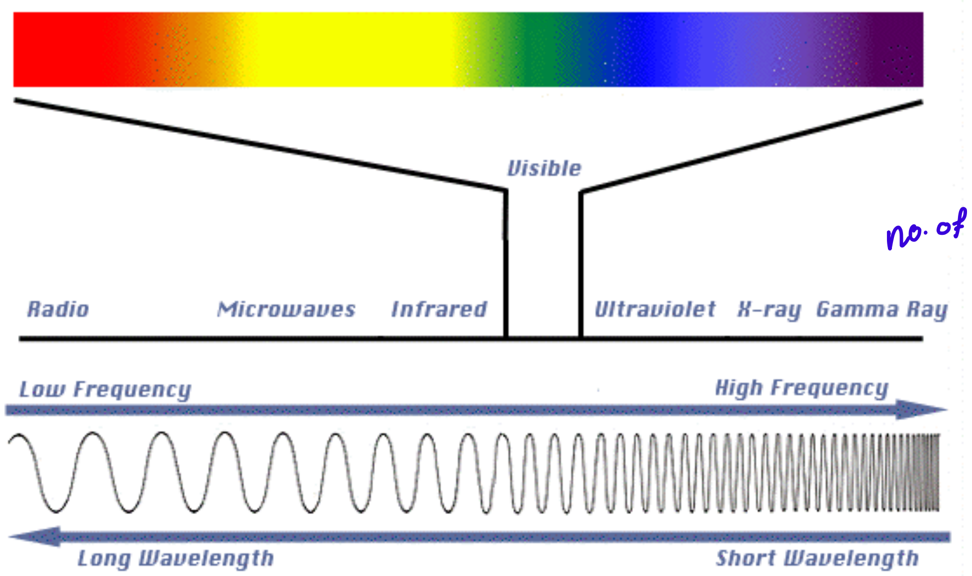
عشان نحضرهم

NMR Spectroscopy

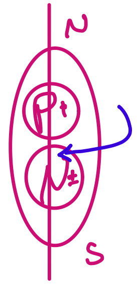
Nucleus

بأي molecule بتلف حول نفسها
إذا اختلف توزيع الكتلة حسب الشكل

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

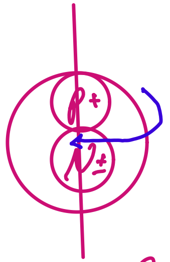


no. of $P^+, N^\pm$



odd

هون ؛
بتوزعوا بطريقة
غير متجانسة وبعملوا
شكل بيضاوي
oval
بينتج عنه أقطاب



even

كيف ما لفنا
بيضلوا متساوين
spherical

اتجاه اللف
α, β

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.

North شمال South جنوب

للتذكير

Nuclear Magnetic Resonance (NMR) Spectroscopy

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

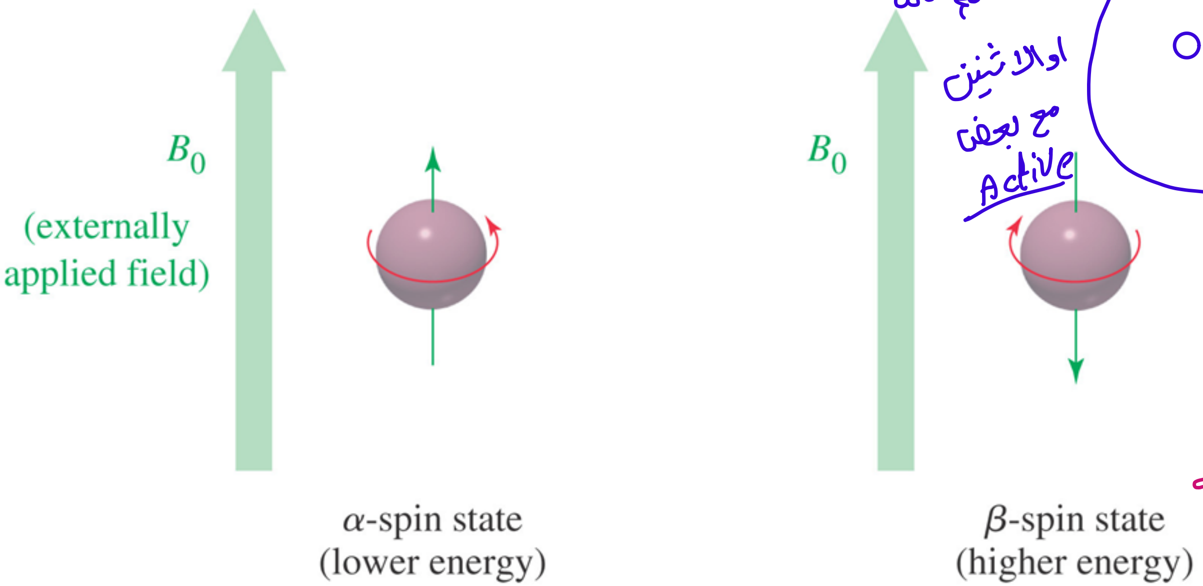
Atomic number = number of (P+)

= number of e^- بالذرة المتعادلة

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

ياواحد منهم odd او الاثنين مع بعض Active

○ even → مابقدر احلله ○ odd → بقدر احلله



Atomic mass = (P+) + (n±)

الكتلة تتركز بالنواة الـ e^- خفيفة

مابتأثر على كتلة الذرة

○ even → Atomic number بشوف ال

even ← مابقدر احلله odd ← بقدر احلله

○ odd → بقدر احلله

atomic mass $\boxed{^{13}C}$

Not all nuclei are suitable for NMR.

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

Natural Abundance

النظائر تختلف بعدد الـ (n±)

^{1}H 99.9% ^{13}C 1.1%

Protium

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

^{2}H Deuterum

H

C

Propan C_3H_8

^{1}H = 99.9%

^{12}C = 98.9%

^{13}C = 1.1%

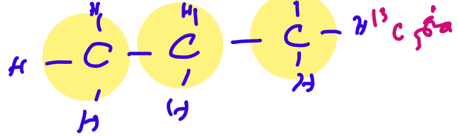
ممكن تكون وحدة H

بقدر احلل كل

H + C

لانه احتمال لكل وحدة من C الموجودة تكون Isomers

^3H Tritium



Nuclear Spin

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

لما اعطي طاقة بيقلب بصير [$S \rightarrow N$, $N \rightarrow S$]

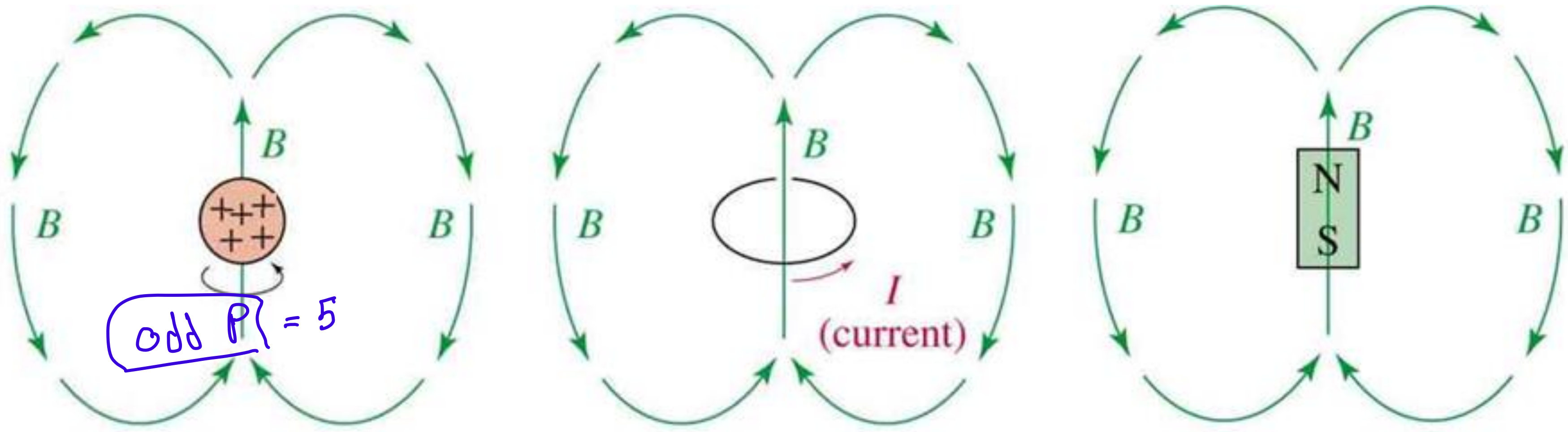
لما يلف حول محور بيعمل مغناطيس

هاي موجبة اكثر

الشحنة

هاد الجانب أثقل

الكتلة



spinning proton

loop of current

bar magnet

لما اوقف الطاقة برجع للوضع الطبيعي

Spectral Properties, Application and Interactions of Electromagnetic Radiation

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

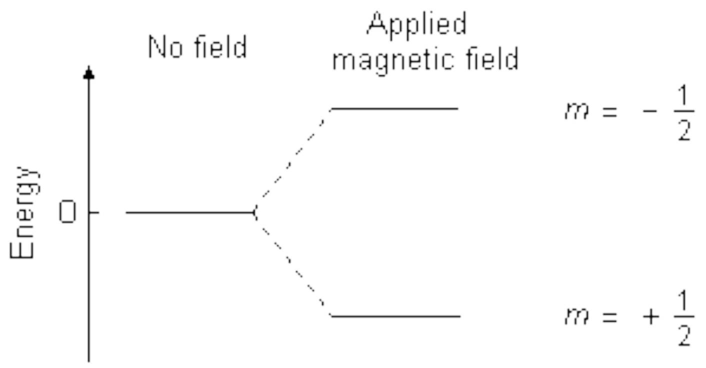
طاقتها قليلة

بين الMicrowave
Radio

Spin Quantum Numbers

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

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



$\boxed{^{13}C}$ ✓

- If the number of neutrons **and** the number of protons are both even, then the nucleus has **NO** spin.
- 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)

no. p = 1
mass = 1
^{1}H

S N
N S

يا بتلف فوق
يا تحت
ولما اسقط الضوء عليها بتقلب
ولما يروح مصدر الضوء بيرجع عالكيف

SPIN QUANTUM NUMBERS OF SOME COMMON NUCLEI

The most abundant isotopes of C and O do not have spin.

isomeres

Element	^{1}H	^{2}H	^{12}C	^{13}C	^{14}N	^{16}O	^{19}F
	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
Atomic Number	odd	odd	even	even	odd	even	odd
Atomic mass	odd	even	even	odd	even	even	odd
Nuclear Spin	✓	✓	✗	✓	✓	✗	✓
Quantum No (I)	1/2	1	0	1/2	1	0	1/2
		$2 \times 1 + 1 = 3$	$2 \times 0 + 1$				
No. of Spin States	2	3	0	2	3	0	2
	up, down						

$2 \times \frac{1}{2} + 1 = 2$

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

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

Table. General rules for determination of nuclear spin quantum numbers

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

P=7 N=8 ← isomer

^{14}N → atom

P=7 N=7

Activ كلهم

Atoms active in NMR

لكن قدرات

الجهاز محدوده

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

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

I = 3/2: ^{15}N

not

Atoms active in NMR

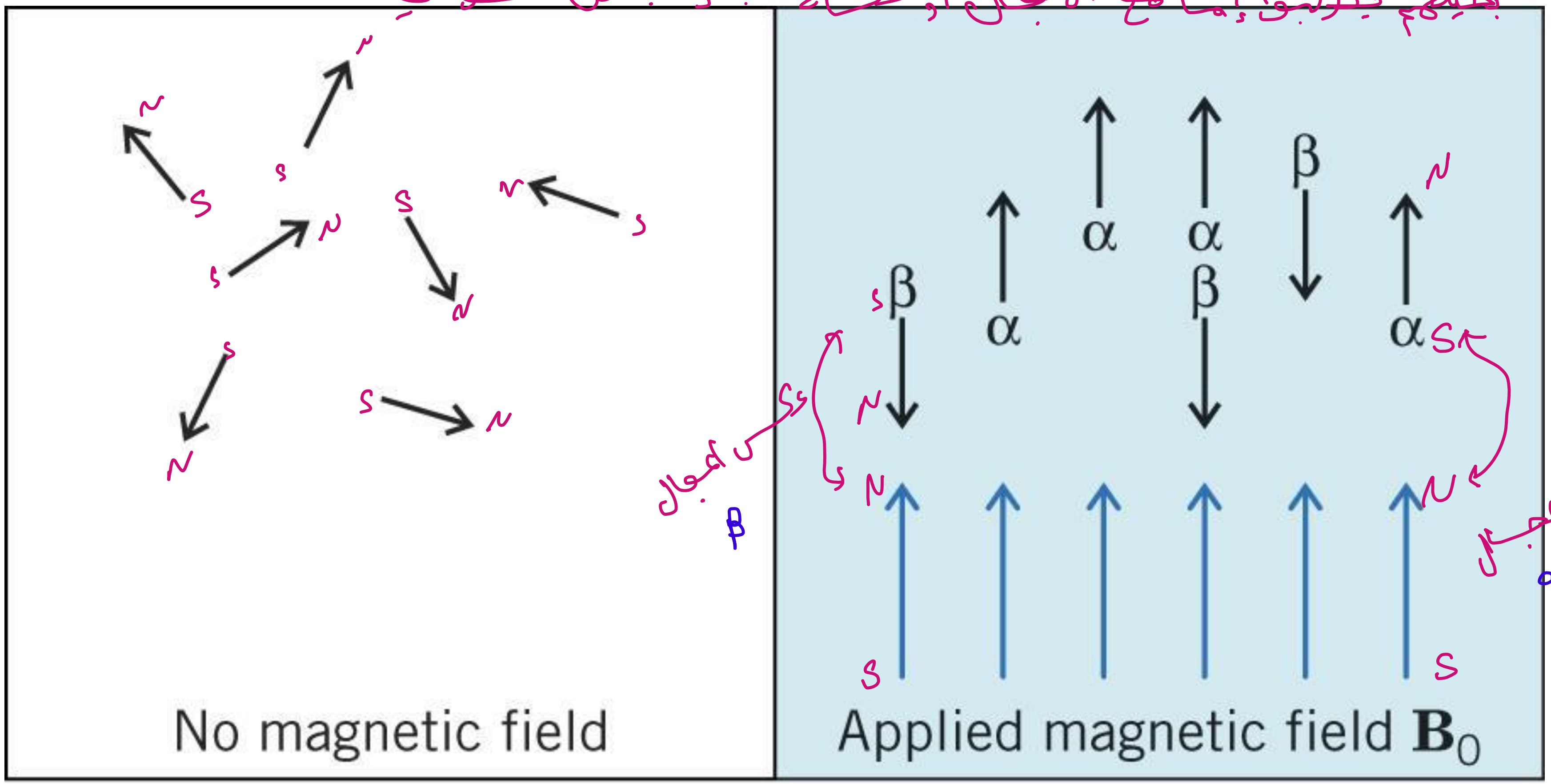
?

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

^{13}C ^{1}H أنوية

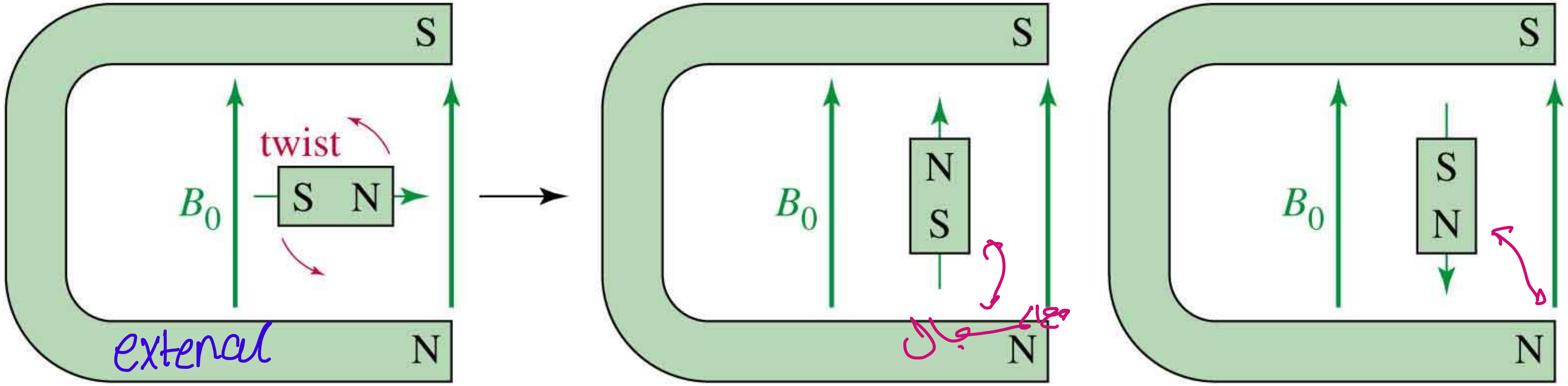
بلفوا بشكل عشوائي

بخليهم يترتبوا إما مع المجال او عكسه



(a) (b)

Behavior of spinning protons with external magnetic field



external magnatic Filede

wave Rang (microwave & Radio)

lower energy
more stable

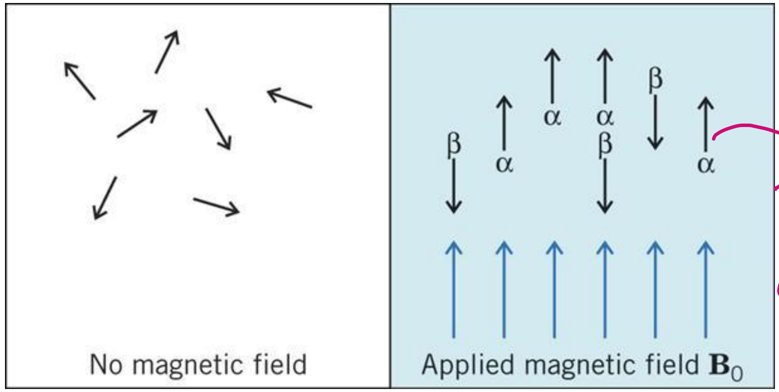
(α-spin state)

higher energy
less stable

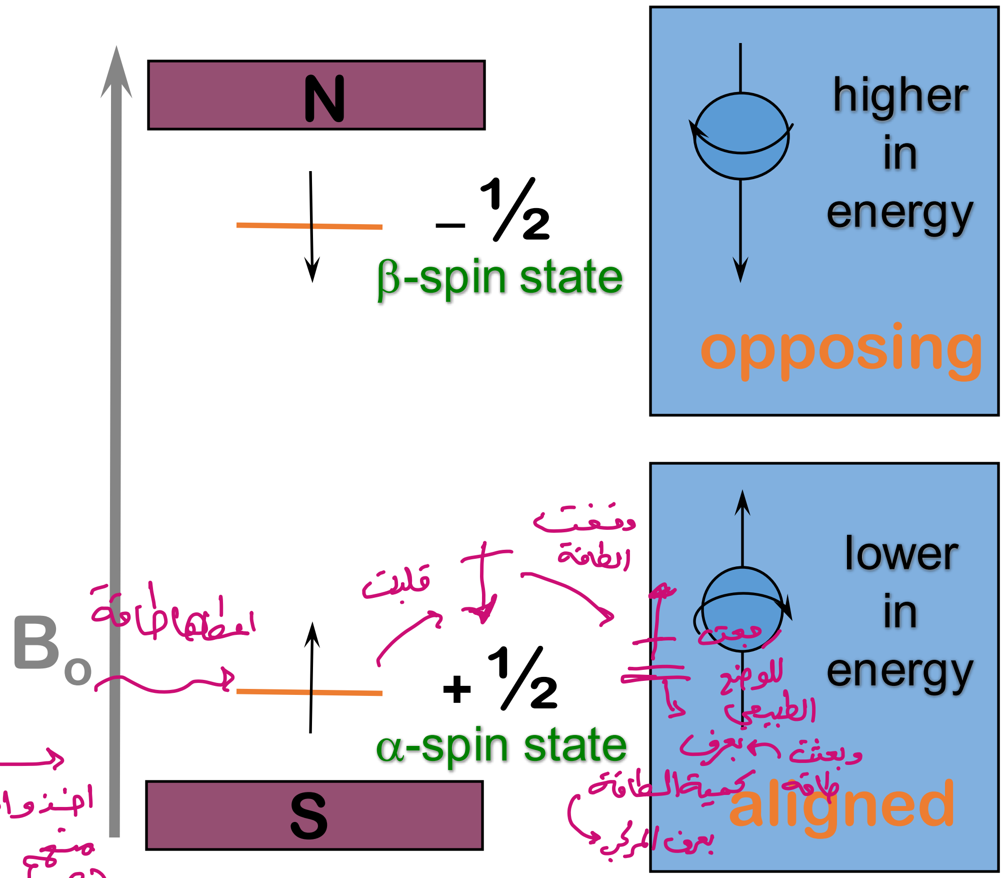
(β-spin state)

الطاقة اللازمة لقلب نواه α = الطاقة اللازمة لقلب نواه β

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.



Nuclear Spin Energy Levels



مرة الـ H ومرة ثانية الـ C مش بنفس الـ Run

In a strong magnetic field (B_o) the two spin states differ in energy

Energy of spinning nuclei

The energy of the nucleus in these two states (orientations) is given by:

gyromagnetic Ratio → spin state

$$\boxed{E = -\frac{\gamma m h}{2\pi} B_0}$$

لانه الحركة دائرية

المجال الخارجي

Energy of α-state (spin aligned)

$$E_{+1/2} = -\frac{\gamma(+\frac{1}{2})h}{2\pi} B_0$$

$$E_{+1/2} = -\frac{\gamma h}{4\pi} B_0$$

Energy of β-state (spin opposed)

$$E_{-1/2} = -\frac{\gamma(-\frac{1}{2})h}{2\pi} B_0$$

$$E_{-1/2} = \frac{\gamma h}{4\pi} B_0$$

Energy difference between the two state

$$\boxed{\Delta E = \frac{\gamma h}{4\pi} B_0 - \left(-\frac{\gamma h}{4\pi} B_0\right) = \frac{\gamma h}{2\pi} B_0}$$

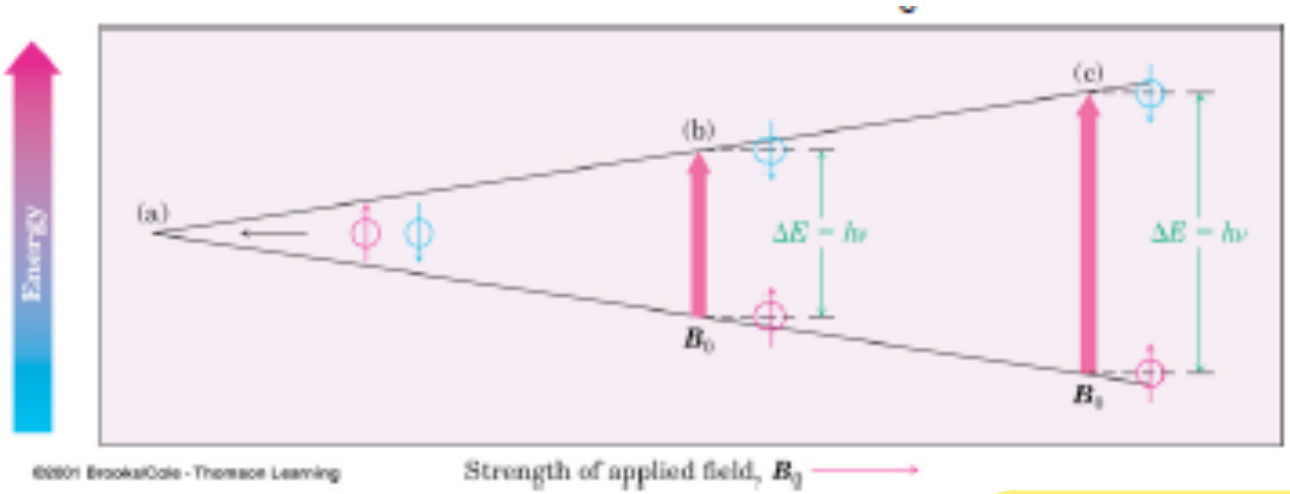
Absorption of electromagnetic radiation of frequency ν that correspond to in energy to ΔE

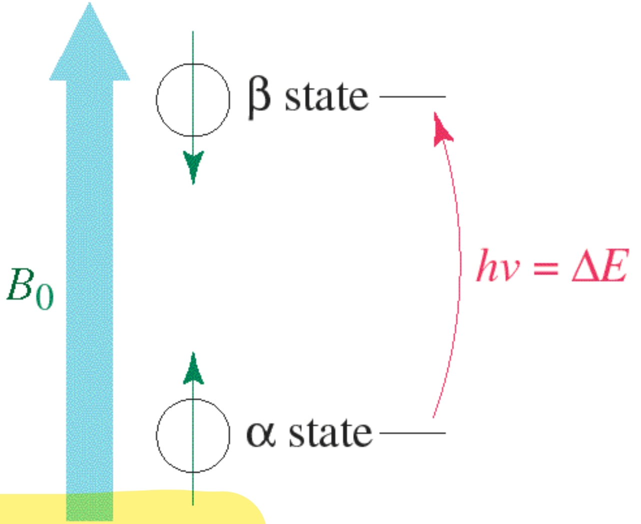
$$\Delta E = \cancel{h}\nu = \frac{\gamma \cancel{h}}{2\pi} B_0$$

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





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

B_o = external magnetic field strength

γ = gyromagnetic ratio

^1H = 26,752 $s^{-1}gauss^{-1}$

^{13}C = 6.7 $s^{-1}gauss^{-1}$

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

. Low energy, radio frequency.

معلومين: * ^{1}H $\nu = 60.025$ gauss

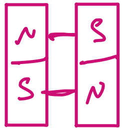
لو قسمناها على 4 ← بعطيني

* ^{13}C $\nu = 15.02$ gauss

Why?

اول سبب ← نواة ال H صغيرة

← قريبين من بعض مشان هيك بدهم طاقة عالية حتى اقدر احلل كل H



بينما نواة ^{13}C كبيرة

بعاد عن بعض فبقدر اقلبهم واحللهم بأقل طاقة من H

السبب الثاني ← Abundance

$^{1}H \Rightarrow 99.9\ \%$ → بدي كمية طاقة كبيرة لانه نسبة ال H كبيرة

$^{13}C \Rightarrow 1.1\ \%$ → بكمية طاقة اقل بقدر احلل لانه وفرتها داخل المركب قليلة على عكس ال H

وبهاي الحالة ال C بستهلك طاقة اقل بكثير من ال H