Nuclear Magnetic Resonance

NMR I

Physical Basis

Ref 9 : (1, 2), 3, 4; 8th ed.

9.: (1), 2, (3), 4; 9th ed.

Also: lab website:
Interactive Tutorials/
NMR Spectroscopy/ Theory

Prob HMWK #2

Adv Rdg 9 : 6, 7; 8th ed.

9 : 7, 8; 9th ed.

General

nmr happens in nucleus of atom

affected by

- surrounding valence e^- 's
- neighboring nuclei

∴ provides info. on

- molecular structure (3D arrangement)
- e^- distribution
- chem. bonding

currently, most important analytical tool in Org. Chem.

Physical Basis

Generally,

- nuclei in atoms are spinning
  (“*nuclear spin*”)
- spinning causes “magnetic moment”
- nuclei behave like little bar magnets

Exception

if (# of p’s) and (# of n’s) are both even ,

then nucleus has no nmr !

Practice

isotope	# of p’s	# of n’s	nmr active ?
^{12}C	6	6	no
^{1}H	1	0	yes
^{2}H	1	1	yes
^{13}C	6	7	yes
^{16}O	8	8	no

this course: **^{1}H only !!**

“ PMR”

Nuclear Spin

^{1}H atom can have

2 different nuclear spin states (m_I)

states α and β have same energy
in absence of mag. field

Effect of External Mag. Field

• put sample inside a magnet

• now states α and β have different energy

• magnet must be very strong
for this effect to be observable

Illustration

effect ....

• transition $\alpha \rightarrow \beta$ possible

if sample is irradiated w/ EMR

that satisfies $\Delta E = h\nu$ (Planck's Equ^n)

• now absorption of energy occurs
• i.e., resonance condition exists

Magnitude of ΔE

depends on

strength of **external** mag. field, B_0;

actually, proportional to B_0

B_0 measured in gauss (G) or

tesla (T)

(1 T = 10^4 G)

current technology uses

1.4 T ——— 14 T (..... 20 T)

magnitude ...

γ, "gyromagnetic ratio",

“nucleus specific”,

determined by experiment

Practice

“PMR” ; B_0 = 1.41 T; ΔE = ?

$\therefore$ very small, indeed

(compare w/ ΔE of chem. rxns, $\approx$100 kJ / mol)

Resonance Frequency, ν_{res}

EMR required to cause

$\alpha \longrightarrow \beta$

(with B_0 — against B_0)

(low E — high E) ?

Ans. : ΔE, ν related by Planck

Previous example cont[d] :

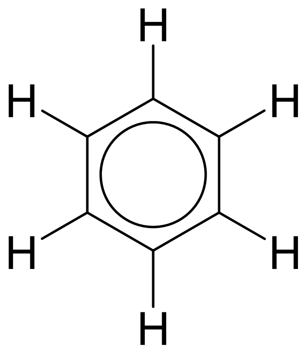
i.e., range of FM radiowaves;

therefore often called **radiofrequency**

App^n to Org. Chem.

cmpd = assembly of nuclear magnets.

e.g.



- any one H could be in α or β state
- any α could be "flipped" to β
  w/ proper radiofrequency
  (= "resonance frequency")

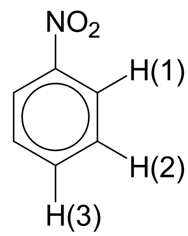
"Clincher"

- NMR would be of little use
  if all H's absorbed ("resonated") at same ν
- differences in "chem. environment",

  i.e., in local e^- density &
  presence of neighboring atoms, esp. H's

  have an effect

Ex.



H(1), H(2), H(3) are different,
∴ resonate (absorb) at different ν values