

Submit a *Single-sided Copy* to the Office

DO NOT STAPLE

no office hours on
Wednesday

1st group office hour on
Thursday (4:00PM)

RECALL: NMR spectroscopy - extremely powerful method for structural analysis

→ Characteristic signal for every type of hydrogen in molecule ("1H NMR")

→ Preclude: Equivalent vs. non-equivalent H's (SECTION 10.8)

KEY TERMS

HOMOTOPIC
ENANTiotopic
DIAStereotopic

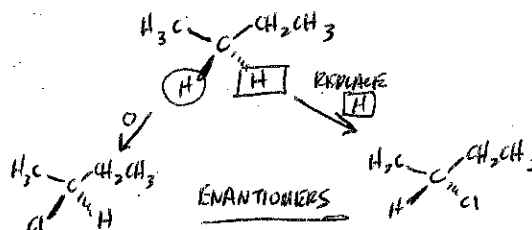
RELATIONSHIPS POSSIBLE
AMONG H'S IN A MOLECULE,
EXAMPLES...

① CH_3CH_3 • All H's ARE EQUIVALENT \Rightarrow 1 SIGNAL IN ^1H NMR

• All H's "HOMOTOPIC"

→ REPLACEMENT TEST - SAME RESULT FROM
REPLACING ANY H BY Cl (FOR EXAMPLES)② $\text{CH}_3\text{CH}_2\text{CH}_3$ - 2 KINDS OF H (CH_3 vs. CH_2) \Rightarrow 2 ^1H NMR SIGNALS- All 6 METHYL H'S ARE HOMOTOPIC CH_3 vs. CH_2 ARE DIFFERENT

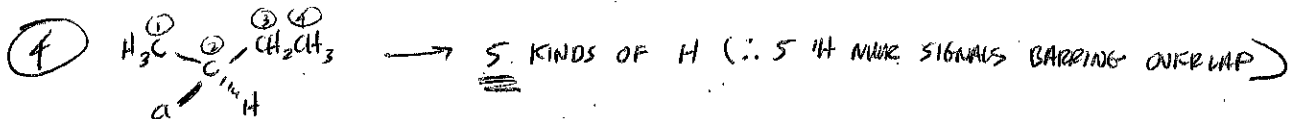
"CONSTITUTIONALLY NON-EQUIVALENT"

- H's ON CH_2 ARE HOMOTOPIC③ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ - 2 KINDS OF H (CH_3 vs. CH_2) \Rightarrow 2 ^1H NMR SIGNALS- All 6 METHYL H'S ARE HOMOTOPICH's ON EACH CH_2 ARE ENANTiotopic

KEY POINT: IN A NON-CHIRAL ENVIRONMENT,
ENANTiotopic H'S ARE EQUIVALENT (SAME ^1H NMR SIGNAL)

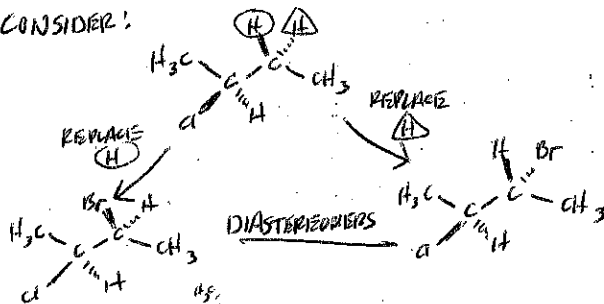
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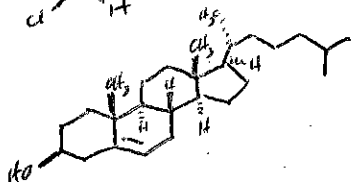


- 3 H'S ON C₁ ARE HOMOTOPIC
- 3 H'S ON C₄ ARE HOMOTOPIC
- CH₃ GROUPS ARE NON-EQUIVALENT (2 DISTINCT CH₃ SIGNALS)
- H ON C₂ IS UNIQUE
- H'S ON C₃ ARE DIASTEREOTOPIC ⇒ NON-EQUIVALENT

CONSIDER:



⑤



36 DIFFERENT KINDS OF HYDROGENS!

- 5 CH₃ GROUPS - All NON-EQUIVALENT (RIGHTMOST CH₃'S ARE DIASTEREOTOPIC)
 - FOR EVERY CH₂ GROUP (11 TOTAL), H'S ARE DIASTEREOTOPIC
- DO THE SUBSTITUTION TEST

WHAT DOES NMR MEASURE?

→ NUCLEAR SPIN. SINCE NUCLEI ARE CHARGED, THEIR SPIN ALLOWS THEM TO INTERACT WITH MAGNETIC FIELDS

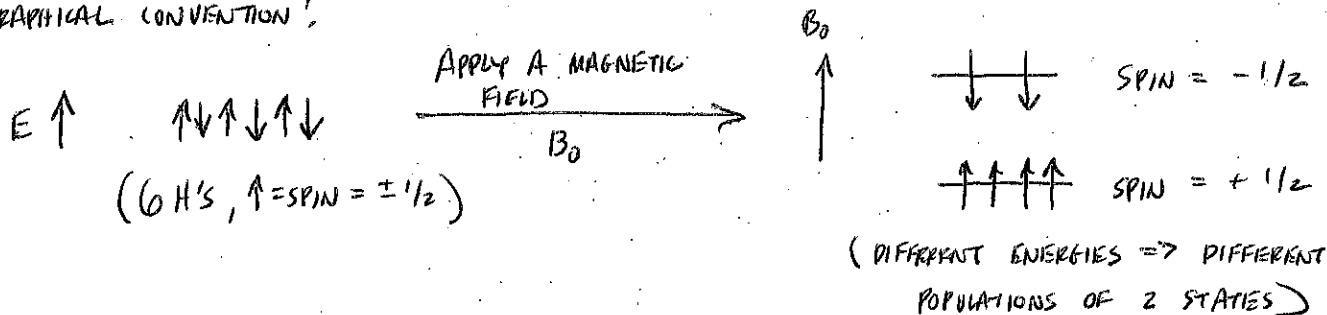
1H: 2 SPIN STATES, "+1/2, -1/2"

→ IN ABSENCE OF AN EXTERNAL MAGNETIC FIELD, THESE STATES ARE INDISTINGUISHABLE (SAME ENERGY)

BUT, IN A STRONG MAGNETIC FIELD, ENERGIES ARE DIFFERENT

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GRAPHICAL CONVENTION:

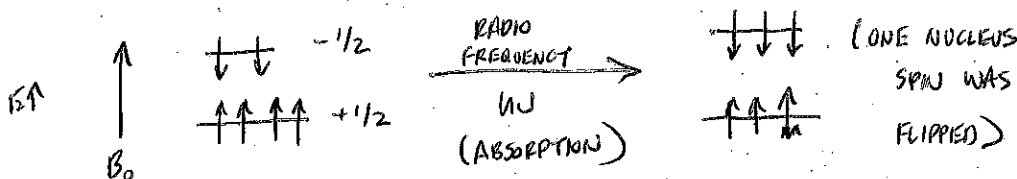


NMR MEASUREMENT - DETECT ENERGY DIFFERENCE BETWEEN 2 SPIN STATES

- THIS ENERGY VALUE IS DISTINCT FOR EACH TYPE OF H IN A MOLECULE

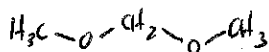
THE ENERGIES REQUIRED FOR A NUCLEAR SPIN FLIP ARE IN RADIO FREQUENCY RANGE

THUS, NMR MEASUREMENT (ONE TYPE OF H):



- THIS ABSORPTION IS REFERRED TO AS "NUCLEAR MAGNETIC RESONANCE"
- THE LOCAL ENVIRONMENT OF A GIVEN TYPE OF H INFLUENCES THE ENERGY REQUIRED FOR NMR ("SPIN FLIP")
- NON-EQUIVALENT H'S EXPERIENCE DIFFERENT LOCAL ENVIRONMENTS, AND THUS UNDERGO SPIN FLIP \Rightarrow DIFFERENT RADIO FREQUENCIES

EXAMPLE (AS IN TEXT)



NOTE: 2 KINDS OF H
CH₃ (6) + CH₂ (2)

¹H NMR SPECTRUM (FIG 13.3)

