

Course Chem 345 Lecturer Gellman
Day Monday Date 1-25-2016
Notes Taken By Lu Liu Total # of Pages 4

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~~To do~~ Recall: ^1H NMR spectroscopy \rightarrow signals for all ^1H atoms in a molecule: VERY powerful for organic molecule structure determination.

Key question - for a given pair (or larger set) of H's
— one NMR signal vs. multiple signals??

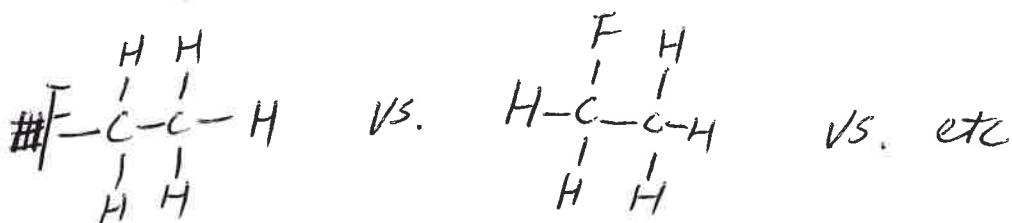
To answer: learn to class H's w/in a molecule as §10.8. Equivalent vs. Non-equivalent (Homo, Enantio & Diastereotopic)

Illustrative examples:

① CH_3CH_3 - All H's equivalent to one another (one ^1H NMR signal)

\dashrightarrow "Homotopic"

"Substitution test"



② Propane $\equiv \text{CH}_3\text{CH}_2\text{CH}_3$

2 kinds of H's — CH_3 vs. CH_2

All 6 methyl H's are ~~enantiotopic~~ ^{Homo} ~~enantiotopic~~. Both methylene H's are ~~enantiotopic~~ & CH_3 H's non-equivalent to CH_2 H's.

HOMOTOPIC

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∴ Predict ^2H NMR signals.

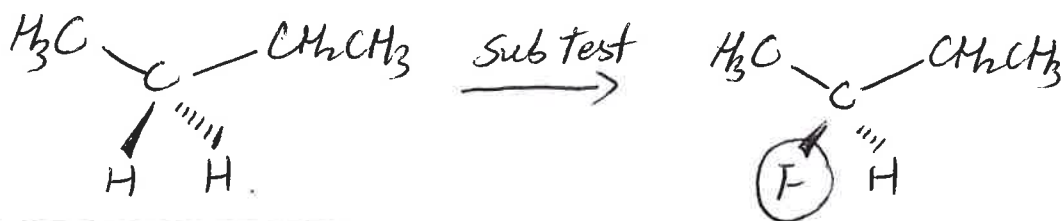
③ Butane = $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$

2 kinds of H, CH_3 vs. CH_2

All CH_3 H's (6) Homotopic.

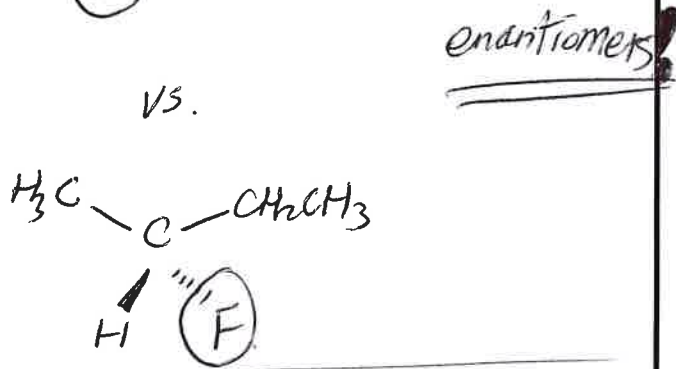
CH_2 non-equivalent to CH_2

H's on each CH_2 are enantiotopic.



Relationship between "enantiotopic"
 & "# of NMR signals"?

If environment (e.g. solvent) is achiral \Rightarrow Enantiotopic H's are NMR equivalent.



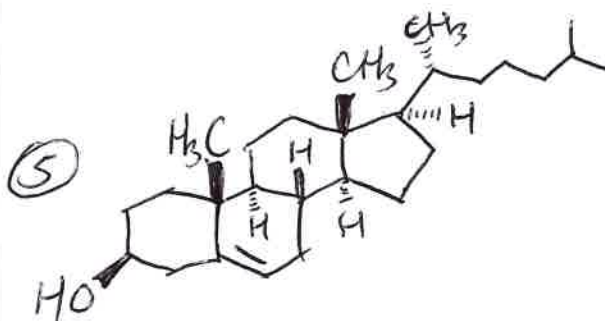
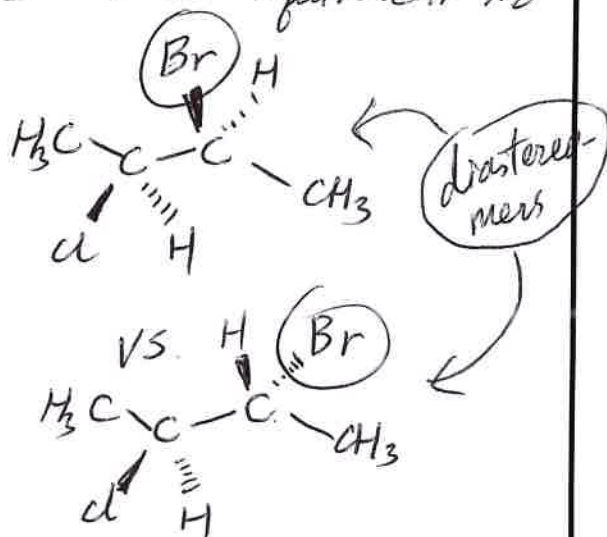
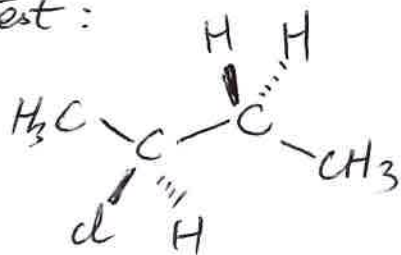
④ $\text{H}_3\text{C}-\underset{\substack{\text{H} \\ \text{H}}}{\text{C}}-\text{CH}_2\text{CH}_3 \Rightarrow$ 5 kinds of H

- 3 H's on C_1 are homotopic
- 3 H's on C_4 are homotopic.
- C_1 H's non-equiv. rel to C_4

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- lone H on C₂ is unique.
 The 2 H's on C₃ are diastereotopic - non-equivalent in ¹H NMR spectrum.

Sub. test:



cholesterol: 36 different kinds of H's!

- 5 CH₃ groups are non-equivalent to one another.

[Note: CH₃'s @ right side are diastereotopic]

- 11 CH₂ groups; in every case, the two H's are diastereotopic.

What does NMR measure?

⇒ Nuclear spin.

Nuclei are charged (+); ∴ spin leads to magnetic field.

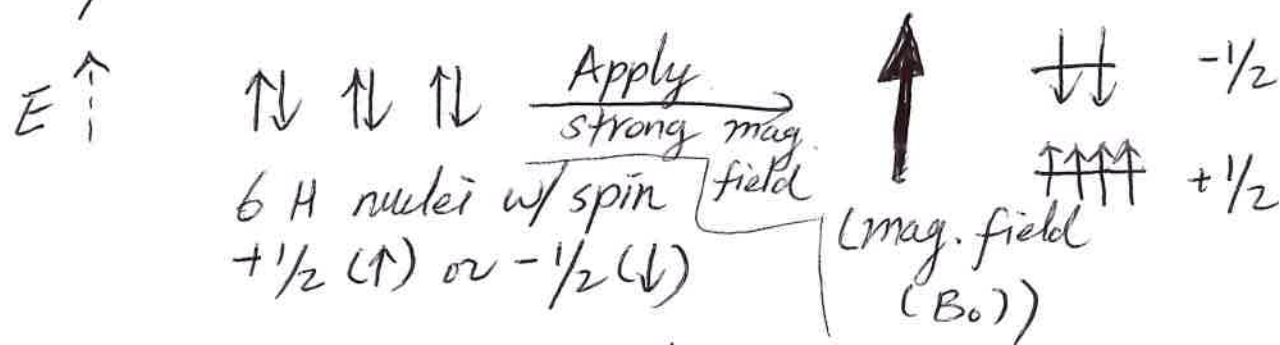
For ¹H nuclei, 2 spin states, +1/2 vs. -1/2

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Usually, these 2 states are indistinguishable (same energy).
 But, in a strong magnetic field, the 2 spin states have
 different energies \rightarrow leads to possibility of NMR

Graphical convention:



NMR measurement — determine energy (radio freq. range) required for "spin flip" of nuclei ($\uparrow \rightarrow \downarrow$)

Abs. of radio freq. radiation by the sample (requires ext. mag. field) — "nuclear magnetic resonance"

Non-equiv. H's w/in a molecule experience different local magnetic environments \rightarrow different energies (spin flip)