

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 a~~ Recall:  $^1\text{H}$  NMR spectroscopy  $\rightarrow$  signals for all  $^1\text{H}$  atoms in a molecule: VERY powerful for organic molecule structure determination.

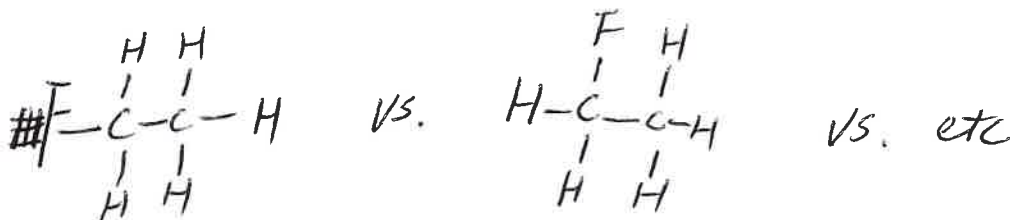
Key question - for a given pair (or larger set) of H's — one NMR signal vs. multiple signals??

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

Illustrative examples:

①  $\text{CH}_3\text{CH}_3$  - All H's equivalent to one another (one  $^1\text{H}$  NMR signal)  $\rightarrow$  "Homotopic"

"Substitution test"



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

2 kinds of H's —  $\text{CH}_3$  vs.  $\text{CH}_2$

All 6 methyl H's are ~~enantiotopic~~ <sup>Homo</sup> homotopic. Both methylene H's are enantiotopic &  $\text{CH}_3$  H's non-equivalent to  $\text{CH}_2$  H's.

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∴ Predict  $^1\text{H}$  NMR signals.

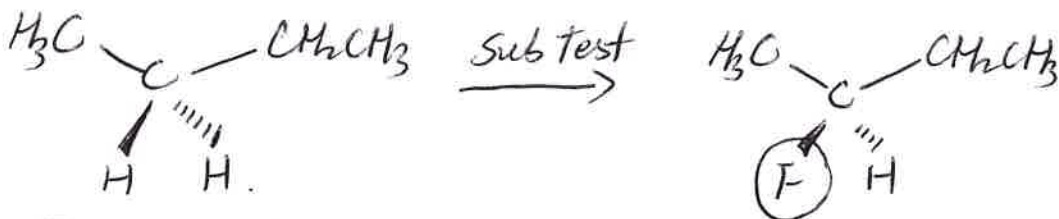
③ Butane =  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$

2 kinds of H,  $\text{CH}_3$  vs.  $\text{CH}_2$

All  $\text{CH}_3$  H's (6) Homotopic.

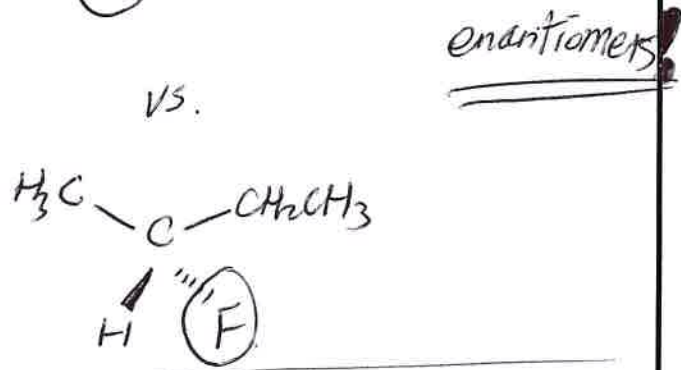
$\text{CH}_2$  non-equivalent to  $\text{CH}_2$

H's on each  $\text{CH}_2$  are enantiotopic.



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

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



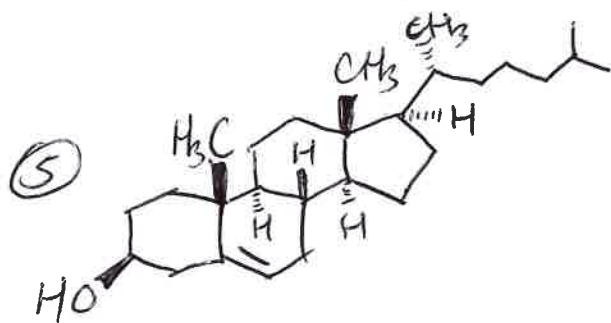
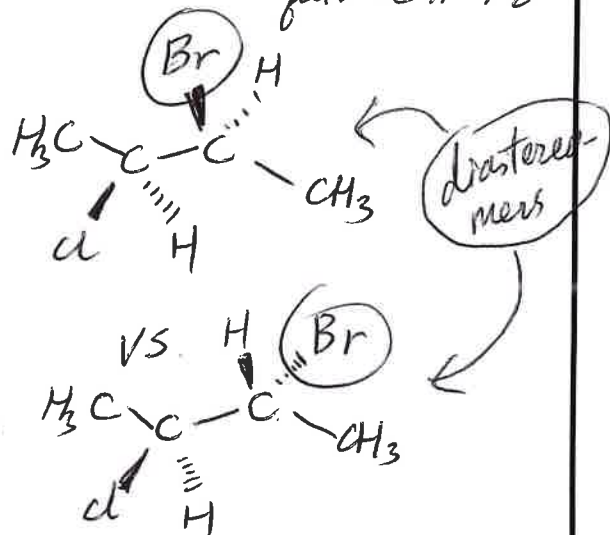
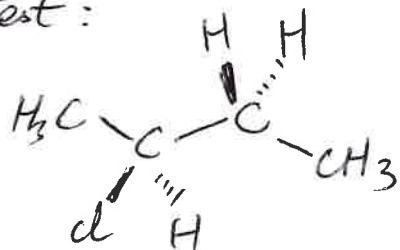
④  $\begin{array}{c} \text{H}_3\text{C} \\ | \\ \text{C} \\ / \quad \backslash \\ \text{H} \quad \text{H} \end{array} - \text{CH}_2\text{CH}_3 \Rightarrow 5 \text{ kinds of H}$

- ① 3 H's on  $\text{C}_1$  are homotopic
- ② 3 H's on  $\text{C}_4$  are homotopic.
- $\text{C}_1$  H's non-equiv. rel to  $\text{C}_4$

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- lone H on C<sub>2</sub> is unique.  
 The 2H's on C<sub>3</sub> are diastereotopic - non-equivalent in <sup>1</sup>H NMR spectrum.

Sub. test:



cholesterol: 36 different kinds of H's!

- 5 CH<sub>3</sub> groups are non-equivalent to one another.

[Note: CH<sub>3</sub>'s @ right side are diastereotopic]

- 11 CH<sub>2</sub> 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 <sup>1</sup>H nuclei, 2 spin states, +1/2 vs. -1/2

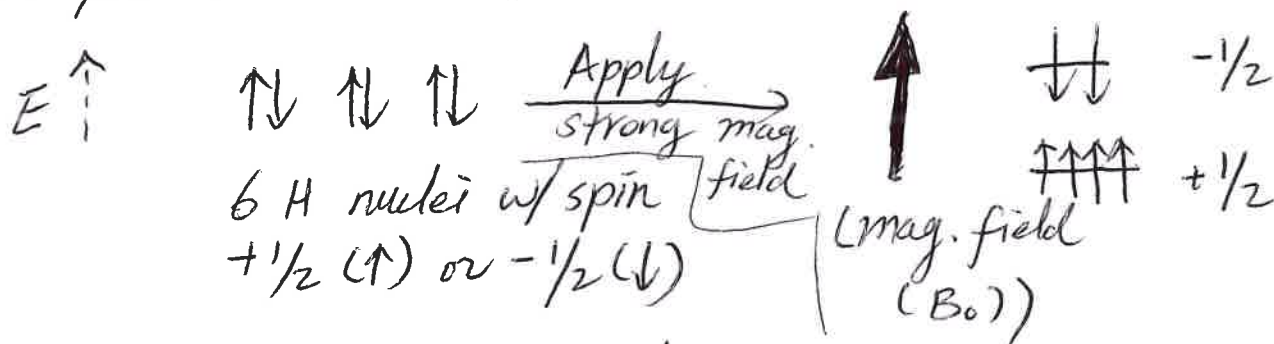


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Usually, these 2 states are indistinguishable (same energy).  
 But, in a strong magnetic field, the 2 spin states have  
 different energies  $\rightarrow$  leads to possibility of NMR

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)