Course Chem 345 Lecturer Grellman

Day Mon. Date 1/26/15

Notes Taken By C. Weatherly Total # of Pages 3

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Formal categories:

homotopic, enantiotopic, diastereotopic - § 10.8 "constitutionally non-equivalent"

Examples: 1) CH_3CH_3 → all H's the same "homotopic"

2) $CH_3CH_2CH_3$ → 2 groups CH_3's, CH_2

NMR... a powerful tool for determining molecular structure.

→ all H atoms contribute to spectrum

Equivalent H's vs. Non-equivalent H's

Equiv. → single ^{1}H-NMR signal

Non-equiv. → different ^{1}H-NMR signals

3) $CH_3CH_2CH_2CH_3$

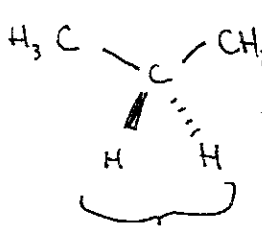
- 2 kinds of H: CH_3, CH_2

→ all 6 CH_3 H's are homotopic

→ CH_3 vs. CH_2 are different

- What about the two H's on a CH_2 group?

→ These are enantiotopic.



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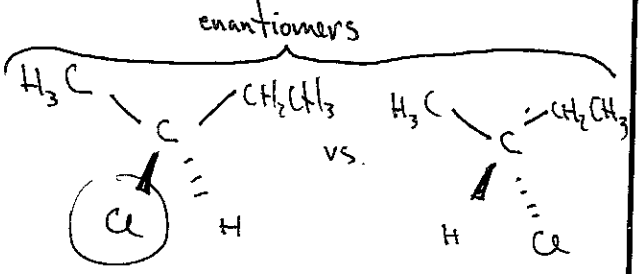

∴ These are enantiotopic.

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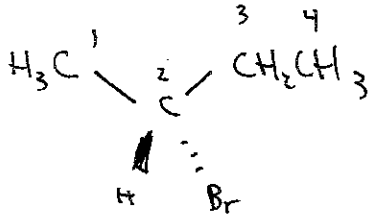
- In an achiral environment, enantiotopic H's are equivalent.

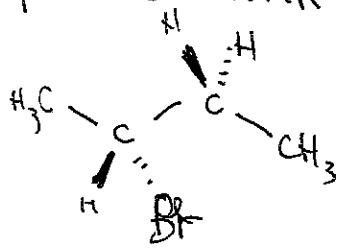
4) Diastereotopic H's



- 5 kinds of H's
∴ Expect 5 NMR signals

- 3 H's on C_1 are homotopic
- 3 H's on C_4 are homotopic
- The two CH_3's are different from one another.
- The H on C_2 is unique.
- H's on C_3 are diastereotopic.
  → non-equivalent under all conditions

Redraw:



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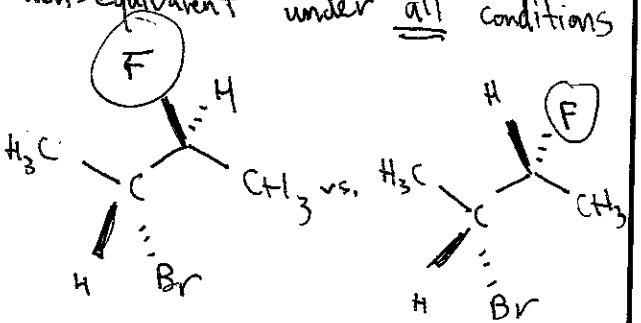
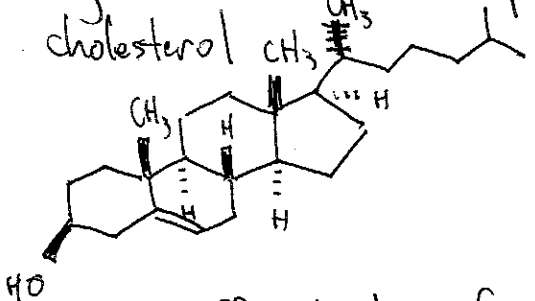


diastereomers

∴ starting H's are diastereotopic

Recall: cholesterol



36 diff. kinds of H's

- 5 CH_3 groups - each is unique (^iPr CH_3's are diastereotopic CH_3 group)
- For every CH_2 unit (11 in all), the two H's are diastereotopic

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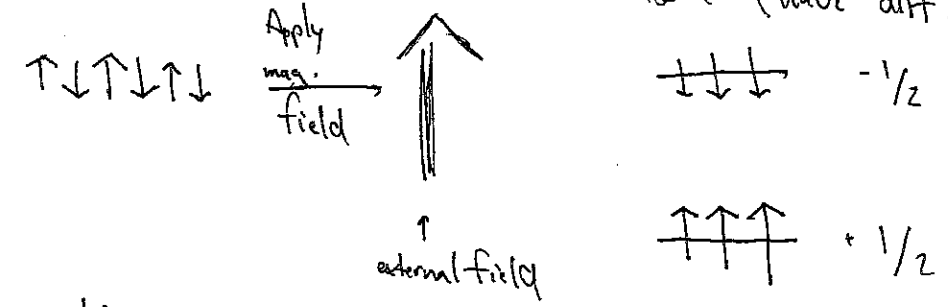
What does NMR measure?
- Nuclear spin.
- Behave as tiny magnets.

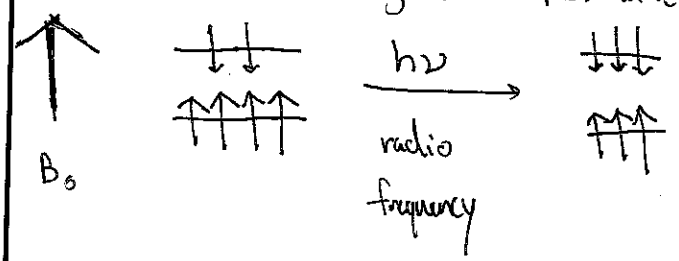
A ^1H nucleus ("proton") has two spin states: $+\frac{1}{2}$ and $-\frac{1}{2}$

→ usually, these two states are indistinguishable (same energy)
Place sample (i.e. the ^1H nuclei) in a strong magnetic field.
Then the two spin states become differentiated (have diff. energies)



↑ ≡ $+\frac{1}{2}$, ↓ ≡ $-\frac{1}{2}$

In this circumstance, the molecule (or "sample") can absorb energy that corresponds to the difference between the $+\frac{1}{2}$ & $-\frac{1}{2}$ states.
"Nuclear Magnetic Resonance"



- Local environment w/in a molecule influences energy required for the "spin flip" transition ∴ Non-equivalents H's have signals at diff. positions in spectrum