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Recall: Use of spectroscopy to learn about molecular structure
- Example: IR — detect specific types of bonds
- Use spectroscopy data to test hypothesis about molecular structure or to formulate a hypothesis

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Chapter 13: Nuclear Magnetic Resonance (NMR) spectroscopy

^1H NMR - signal for every type of H in molecule

^{13}C NMR - every type of ^{13}C in molecule

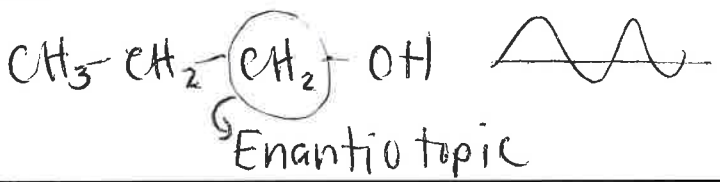
Rec. Problems: 3, 6-28, ~~#~~ 31-47, 52, 53, 55-59

Equivalent H's vs. non-equivalent H's
→ All equivalent H's in a molecule contribute to the same NMR signal ("resonance").

Relationships among H's in a molecule:
- Homotopic
- Enantiotopic
- Diastereotopic

} Section 10.9

Consider:



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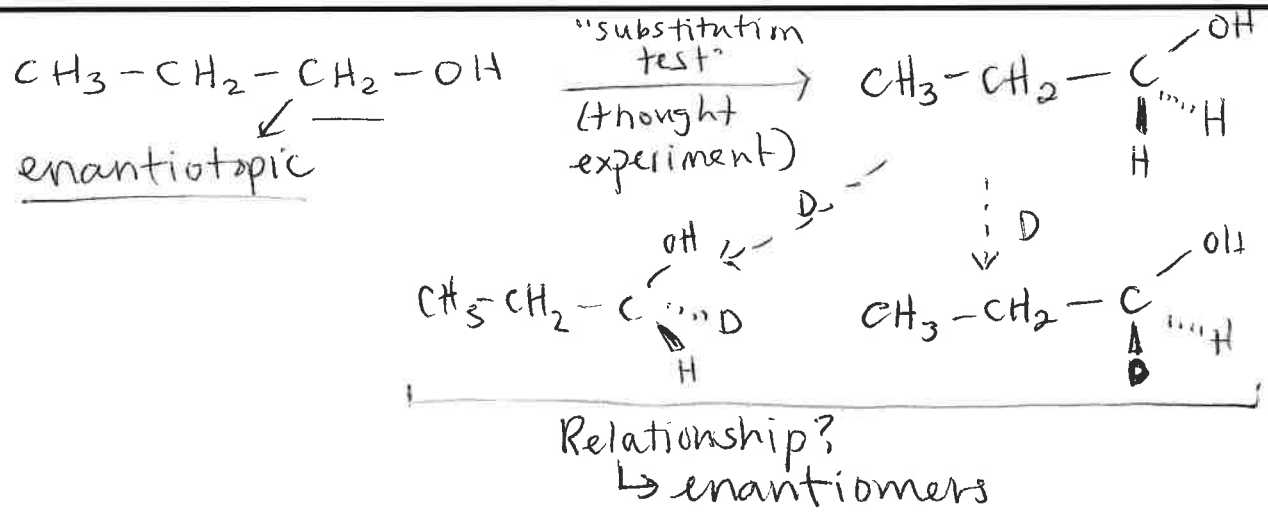


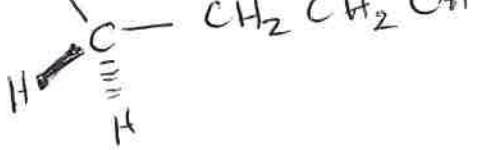
$CH_3CH_2CH_2OH$

↳ also enantiotopic

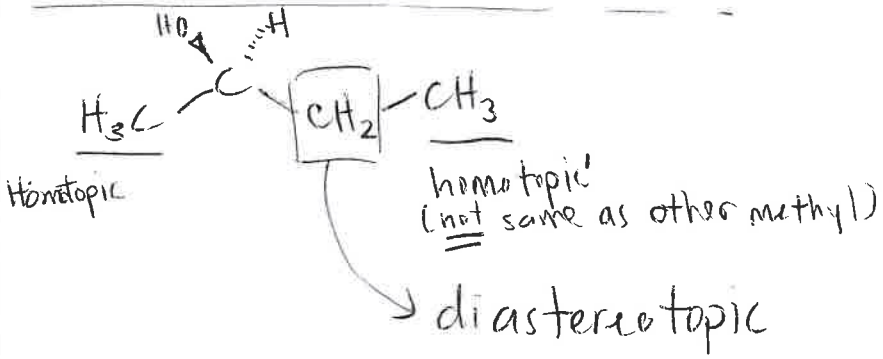
prove this to yourself

$CH_3CH_2CH_2OH$

↳ homotopic — substitution test



NOT creating a chiral center w/ "substitution test"



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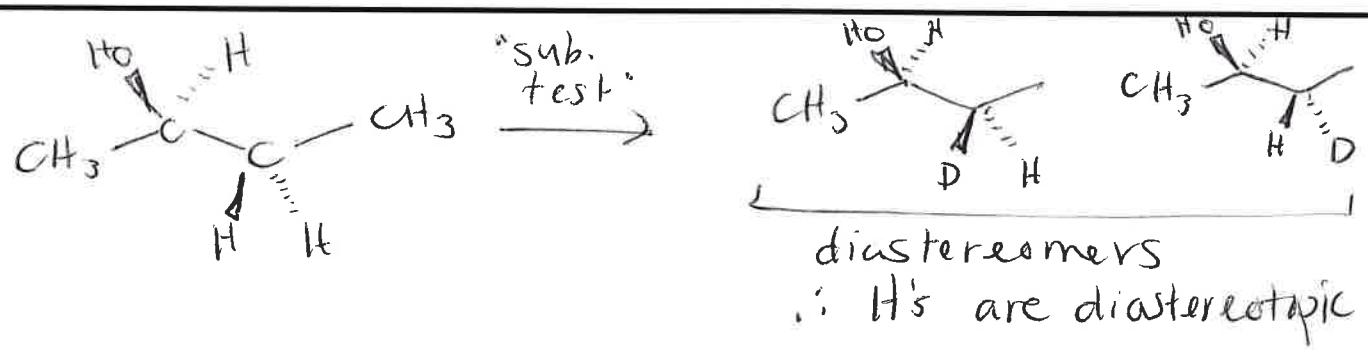


∴ H's are diastereotopic

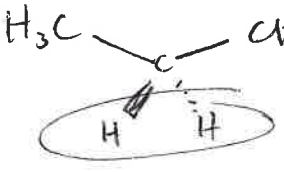
Equivalent vs. non-equiv. H's – EXAMPLES

(1) CH_3CH_3 All H's equivalent
⇒ single ^1H NMR resonance (all 6 H's)

(2) $CH_3CH_2CH_3$ All methyl H's equivalent to one another (6 total)
Both CH_2 H's equivalent to one another (2 total)
⇒ 2 ^1H NMR resonances

Note: All 6 CH_3 H's are homotopic, homotopic H's are equivalent to one another

(3) $CH_3CH_2CH_2CH_3$ 6x methyl H's – homotopic
∴ one resonance
4 x methylene (CH_2) H's – [redacted]
are ... ?
let's see!

Consider: 

enantiotopic

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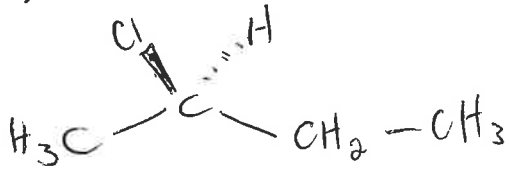
enantiotopic H's are equivalent in terms of NMR in an achiral environment

Most solvents you are used to are achiral!

All 4 CH_2 H's in ~ are NMR equivalent

⇒ ^1H NMR spectrum of ~ has 2 resonances

(4)



5 ^1H NMR ~~signals~~ signals

(i) H_3C @ C_1

(ii) H_3C @ C_4

(iii) H ~~@~~ @ C_2 (bearing Cl)

(iv) ½ (v)

diastereotopic ⇒ NMR equivalent

Sometimes diastereotopic H's will accidentally overlap. But purely coincidental

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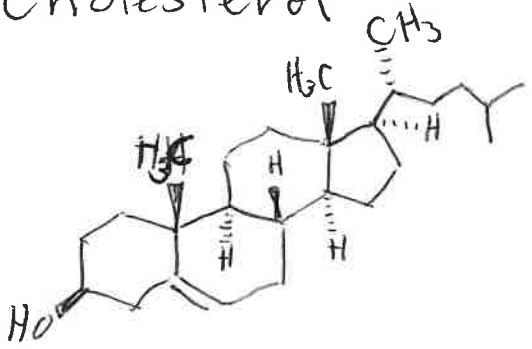
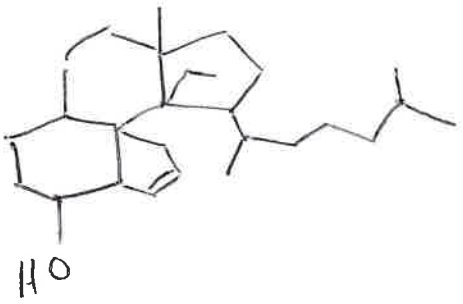
Cholesterol



36 different kinds of H's

Proposed structure (1928)



What ~~are~~ do we measure by NMR ?

→ Nuclear spin

remember that there are relationships ~~bet~~ between charged entities & mangnetic fields