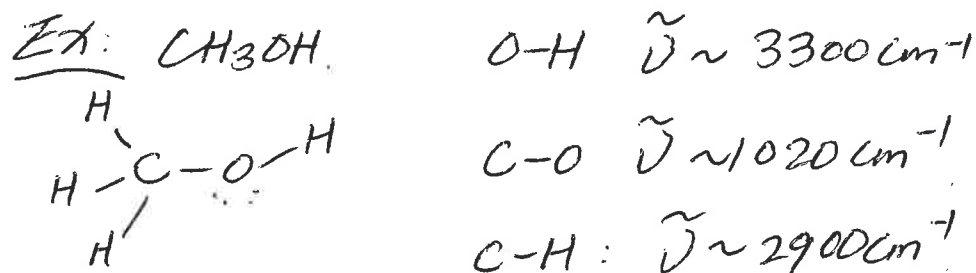


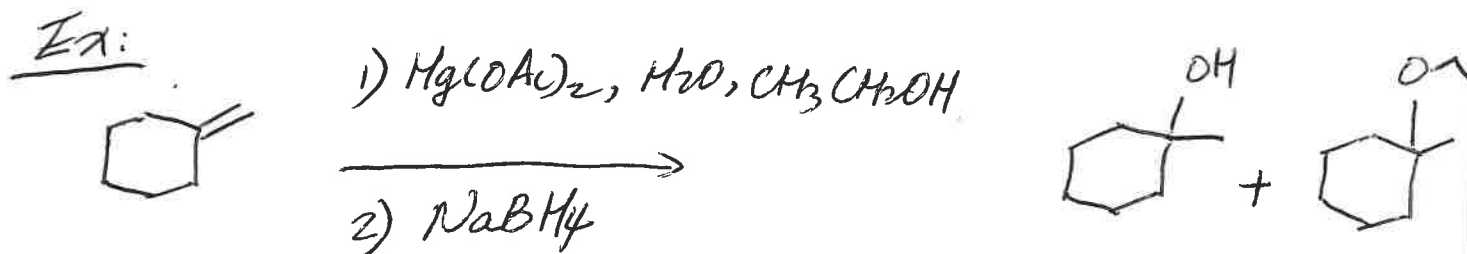
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Recall: IR spectroscopy. } Information of  
 → Internal motions w/in } particular bond types  
 molecules (e.g. bond stretching) } ~~at~~ & functional  
 groups.



How does one use IR data to deduce structures of organic molecules? → Test of structural hypotheses; discriminate between alternatives



products ~~&~~ separated ... but which is which?

Know: RO-H has strong ~~signal~~ IR signal

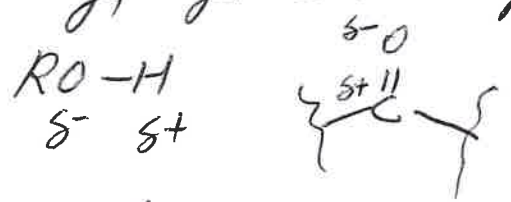
Logic: only one of expected products has -OH group.

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Which types of bonds have useful IR signals?

(What is "useful" here?)

1) strong signal — highly polar bond



2) signal occurs in an "uncrowded" region of IR spectrum ( $\geq 1500 \text{ cm}^{-1}$ )

3) Bond type should not be too common (seek distinctive characteristic info).

Consider: C-H bonds

C(sp<sup>3</sup>)-H: 2850-2950 cm<sup>-1</sup> Too common - <sup>not</sup> diagnostic

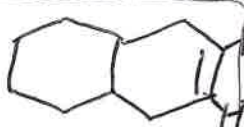
C(sp<sup>2</sup>)-H: 3000-3100 cm<sup>-1</sup> } very diagnostic

C(sp)-H: ~3300 cm<sup>-1</sup>

How distinguish:



vs.



→ Alkene reactivity  
 H (takes time/days)

vs.

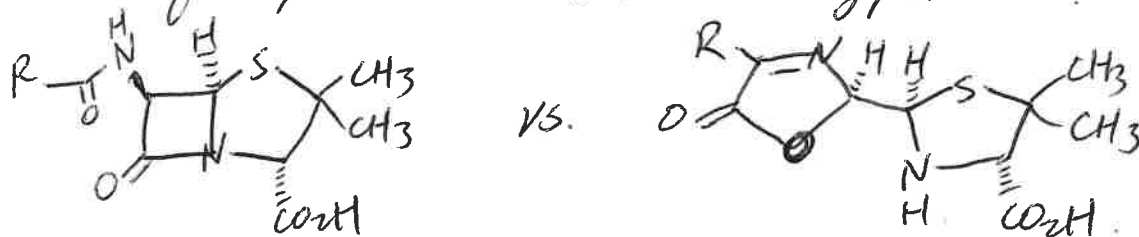
IR spectrum signal

3000-3100 cm<sup>-1</sup> ⇔ Alkene

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Historical Example (early 1940s)  
structure of penicillin(s): Two hypotheses.



Recommended bk: *The Enchanted Ring* by J.C. Sheehan  
Chap. 13 - Nuclear Magnetic Resonance (NMR)  
spectroscopy.

→ The most powerful structural technique for  
organic chemists!

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

Focus on atomic nuclei:

Most common:  $^1\text{H}$  NMR ("proton" NMR)

→ signals for all H atoms in a molecule.

Also useful:

$^{13}\text{C}$  NMR

Crucial Concept: Equivalent vs. Nonequivalent H's  
(or C's)

⇒  $\frac{1}{5} \times 10.8$

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Equivalent H's give rise to a single NMR signal;  
non-equivalent H's give rise to different NMR signals.

Key terms: Relationships between H's w/in a molecule.

Homotopic

Enantiotopic

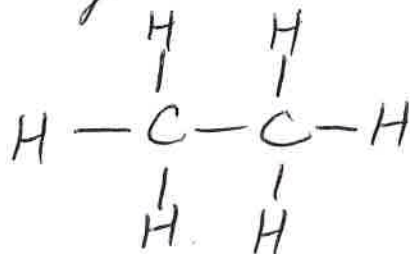
Diastereotopic

("Different" or "constitutionally non-equivalent")

Examples:

①  $\text{CH}_3\text{CH}_3 \Rightarrow$  All 6 H's are homotopic. One "H NMR" signal. i.e., the 6 H's are all "equivalent" to one another from the NMR perspective.

Analysis — "Substitution test" (thought expt.)





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

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

- All 6 H's on  $\text{CH}_3$ 's are homotopic

-  $\text{CH}_3$  H's are const. non-equivalent to  $\text{CH}_2$  H's  
H's on each  $\text{CH}_2$  are enantiotopic relative to one another.

