Course Chem 345 Lecturer Gellman

Day Friday Date 1/23/15

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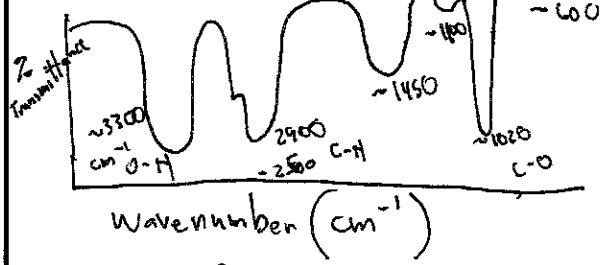
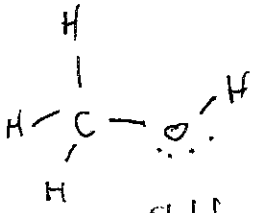
Guest Lecture by. Chari Barta

IR spectroscopy

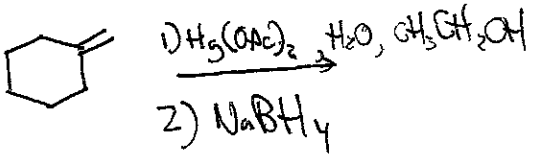


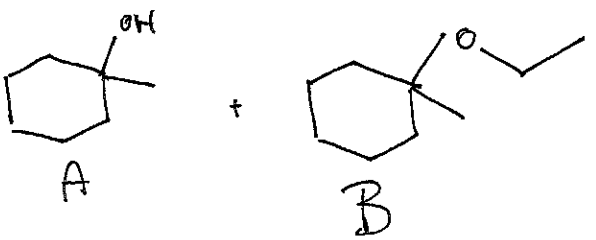


Sketch of CH_3OH spectrum.

* Why IR?
  1) evidence for or against specific types of bonds / functional groups
  2) allows us to determine between alternative hypotheses for structure of a given molecule

A familiar reaction:





R O - H → expect strong IR absorption (3200 - 3400 cm^{-1})

* Sample w/ abs. 3200 - 3400 cm^{-1} ⇒ A
* Sample w/o " " " " ⇒ B

Qualities that make IR useful:

① strong signal (prominent in spectrum) (polar molecules tend to give stronger signal)

② peaks in uncrowded region of IR spectrum

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- organic chemists focus on: 3600 - 1500 cm^{-1} - uncrowded region
  [$\leq$ 1500 cm^{-1} - peaks are nearly unassignable]
  (1000 cm^{-1} acc. to some)

(3) Bond type that isn't too plentiful

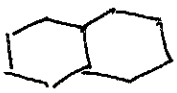
Ex. sp^3 C-H stretches : 2850-2950 cm^{-1}

sp^2 C-H " : 3000-3100 cm^{-1}

sp C-H " : 3300 cm^{-1}

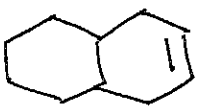
- since ~~virtually~~ ~~all~~ most organic molecules contain sp^3 C-H bonds, little information available in 2850 - 2950 cm^{-1}

Ex.



X

vs.



Y

Which is which?

- both has abs. 2850-2950 cm^{-1}
- only Y has abs. 3000-3100 cm^{-1} (sp^2 C-H stretch)

- Before development of IR, had to test for reactions

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Chap. 13: Nuclear Magnetic Resonance (NMR) Spectroscopy
* Most powerful analytical tool for most organic chemists!

Rec. problems: 3, 6-26, 30-46, 48, 49, 51-58

- Method focuses on atomic nuclei
- detects all nuclei of a given type in a molecule
- organic chemists: most common NMR spectroscopy → ^1H "proton-NMR"
  - ^{13}C-NMR is also useful
  - ^{31}P, ^{19}F, others are occasionally useful

^1H-NMR - signal for each type of H in a molecule
- critical concept for ^1H-NMR interpretation

⇒ all equivalent H's contribute to a single NMR signal
⇒ non-equivalent H's (or sets of non-eq. H's) give rise to different NMR signals.

——→ Re-read sec. 10.8 in London text.
* homotopic: chemically equivalent groups
* enantiotopic: chemically non-eq. groups w/in a chiral environment. → are chemically equivalent out of a chiral environment
* diastereotopic: chemically non-equivalent groups

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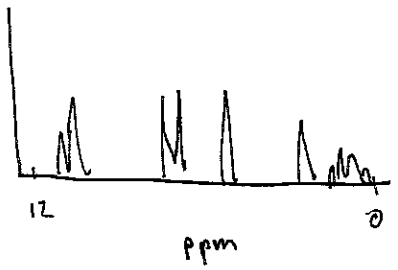
Examples:

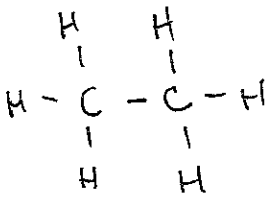
Sample NMR spectrum:



How many chemically distinct protons:

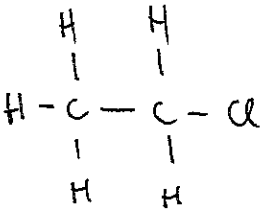
1) CH_3CH_3

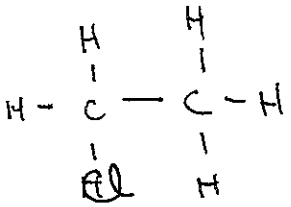
* All equivalent
* One NMR signal



To see, try a substitution test.

1) Replace a proton w/ another atom.
2) Replace another





The molecules are the same! So the H's are chemically equivalent.

- This test is an exercise on paper. No actual reactions need to be done.

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(2) $CH_3CH_2CH_3$ (plane of symmetry)

* 2 ^{1}H-NMR signals
* 2 kinds of H's (CH_3 vs. CH_2)

- all 6 methyl H's are homotopic
- middle (methylene) H's are homotopic
- CH_3, CH_2 ⇒ constitutionally non-equivalent

(3) $CH_3CH_2CH_2CH_3$ ⇒

* 2 ^{1}H-NMR signals
* 2 kinds of H's (CH_3 vs. CH_2)

- all 6 methyl H's are homotopic
- CH_3, CH_2 are different
- H's on a CH_2 are enantiotopic

Sub. test: