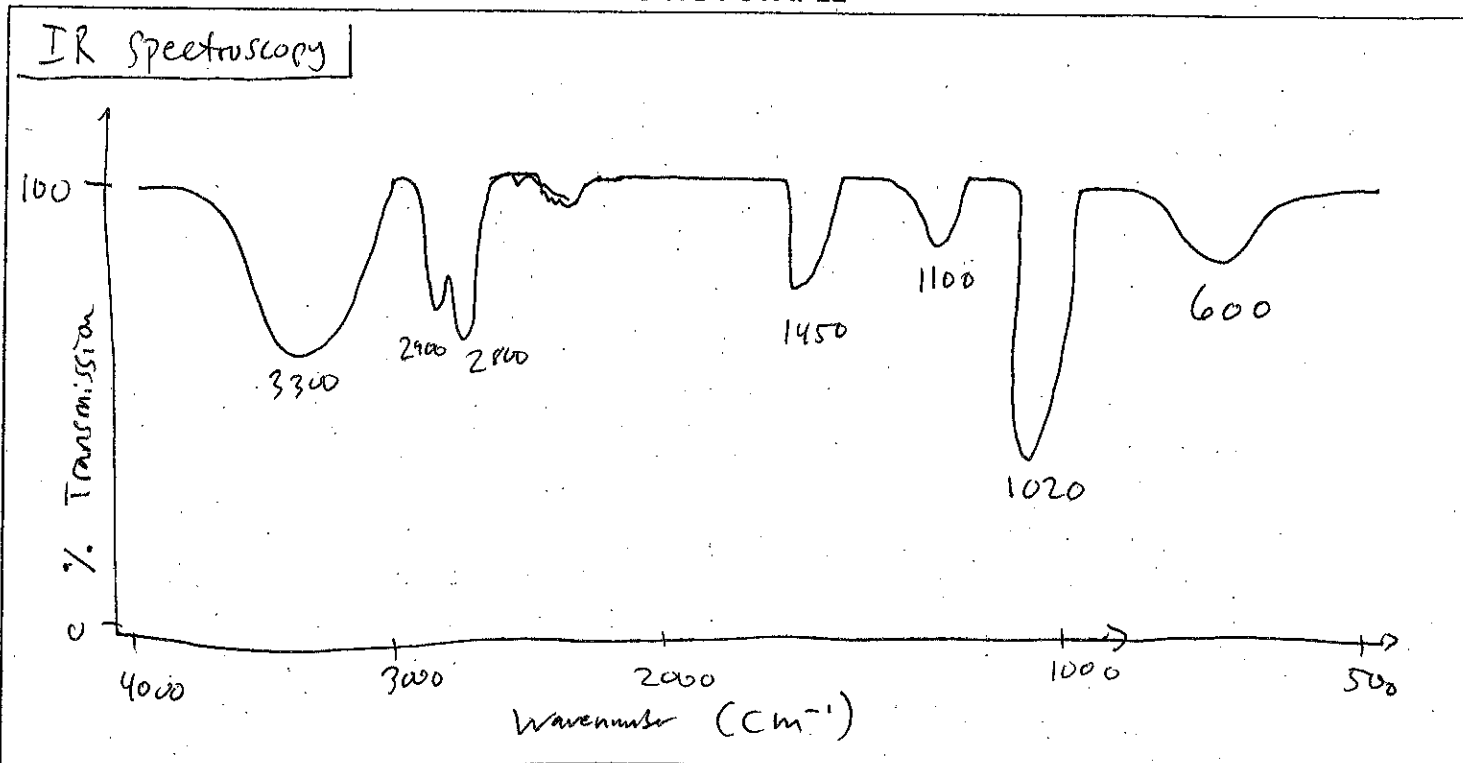


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Horizontal scale is $\tilde{\nu} = \frac{1}{\lambda}$ ("wavenumber")

How do we interpret these data?

$\sim 3300 \text{ cm}^{-1}$ O-H stretch

$\sim 2900 \text{ cm}^{-1}$ C-H stretch

$\sim 1000 \text{ cm}^{-1}$ C-O stretch

① How do we know this? How do we make these assignments of a wavenumber to a particular functional group?

→ Consult an IR table (always provided for you on exams)

London Table 12.2, Appendix 2

Don't need to assign all signals, only the key ones.

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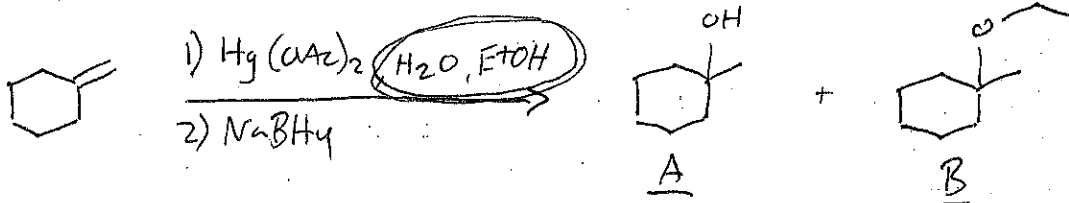
② Other signals?

→ Don't know what these are. OK to ignore for our purposes

③ How do we make use of IR data?

→ Evidence for specific bond types (functional groups)

For example: discriminating between or among alternative structural hypotheses.



Imagine we isolate two separate products. How do we know which is which?

From IR table, we know that OH stretch should be $3200 - 3400 \text{ cm}^{-1}$
no other bands should be in this region.So, if we observe a 3250 cm^{-1} band in one, and no band $> 3000 \text{ cm}^{-1}$
in the other, then the first must be A and the second B.

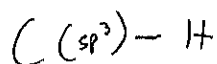
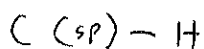
Qualities that make IR signals useful

- ① Strong (prominent): Polar bonds tend to have stronger signals (e.g. C-O or O-H)
- ② Occurs in an uncrowded region of the spectrum. We tend to focus on the region $> 1500 \text{ cm}^{-1}$
- ③ Bond types that are not common. For example... →

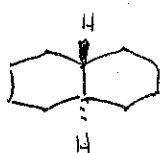
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Consider 3 types of C-H bonds

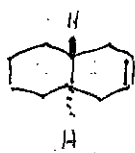
2850-2950 cm^{-1} ← COMMON. Expect to see
in pretty much everything3000-3100 cm^{-1} } less common, more
useful for figuring out
structural information3300 cm^{-1}

For example:



A

+

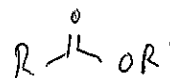
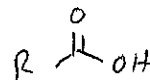
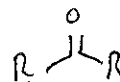
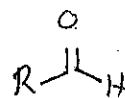


B

In the old days (pre-1950), ~~was~~
could test which ~~one~~ reacts with
 H_2 and Pd/C. But this requires
 ≥ 1 day and uses ~~you~~ up your
compound.

Instead, using IR, we can look for the sp^2 C-H stretch
around 3000-3100 cm^{-1} to identify B. Takes < 5 min and is non-destructive.

IR is very useful for identifying carbonyl groups, e.g.



etc.

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Nuclear Magnetic Resonance (NMR) SpectroscopyLondon ch. 13. ~~Problems~~ Problems: 3, 6-26, 30-46, 48, 49, 51-58.NMR is the most important analytical tool for organic chemists.

Focusing on the nuclei themselves, rather than the bonds between them we can detect all the different kinds of a given nucleus in a given molecule. In particular, we usually look at H (^1H in particular) and C (^{13}C in particular).

Preludes: Equivalent vs. non-equivalent hydrogens (or carbons)This is an ~~essential~~ essential concept to understand for NMR.All equivalent ^1H 's contribute to a single signal ("resonances")All non-equivalent ^1H 's give rise to different signals (which sometimes are overlapping)Critical: Read London 10.8Important Terms:

homotopic

enantiotopic

diastereotopic

} possible relationships among ^1H 's within a single molecule.Illustrations/Examples: ① CH_3CH_3 All ^1H 's are equivalent

one NMR signal

These ^1H 's are "homotopic"