Overheads: - Outline, NMR Bruice

Recap Monday:

Mass Spectrometry:

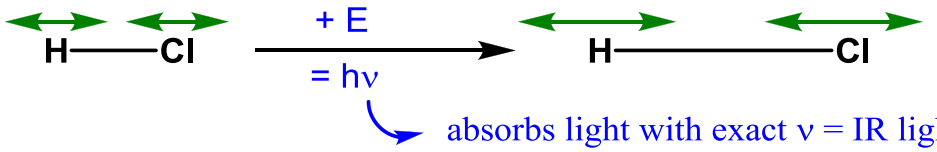
M^+ = Molecular weight (⇨ formula) = highest mass peak

Fragments: most stable cations biggest (most abundant)

- Characteristic of functional groups
- Best used to confirm structure

Infrared (IR) Spectroscopy

- Vibration of bonds



absorbs light with exact ν = IR light

Downward peaks in spectrum mean less light passing through

- Position depends on: - atoms in bond
  - strength of bond

Hooke's law: (for spring)

$$\bar{\nu} = 4.12\sqrt{\frac{f}{\mu}}$$

f = force constant relates to bond strength (≡ > = > -)

μ = reduced mass = $\frac{M_1M_2}{M_1+M_2}$

$\mu \uparrow$ if $M \uparrow$ $\therefore \bar{\nu} \downarrow$ for heavier atoms

Characteristic Functional Groups:

Figures 14.13 carbonyl (C=O): 1800-1650, usually strongest peak
→ Exact value depends on type of C=O

14.14a-b alcohols (O-H): 3650-3200, very broad, strong
NOTE: fingerprint region: < 1600

14.19 vs 14.20 (RCO_2H: 3300-2500, extremely broad)

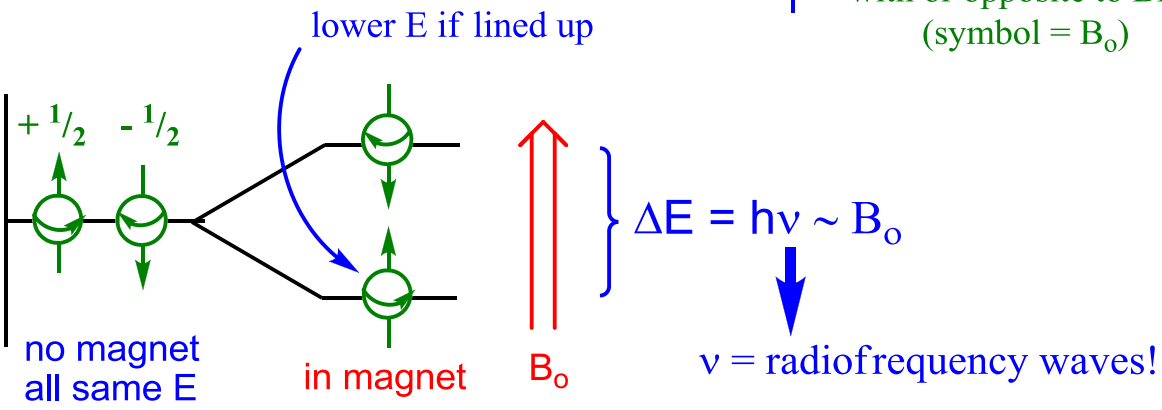
14.25 amine (N-H or NH_2): 3500-3300, medium
→ less broad than OH (less H-bonding)
→ 2 peaks if NH_2

Table 14.4/13.4 gives IR frequencies

NMR Spectroscopy

Nuclei of some atoms (including ^1H) have "spin"

- like spinning top
= moving charge ∴ like tiny magnet
- if put into "BIG" magnet, line up with or opposite to BIG magnet
(symbol = B_o)



Key Point: electrons also tiny magnets (moving – charge)
→ line up opposite to B_o
→ come between nucleus and BIG B_o
∴ electrons "shield" nucleus from B_o, so actual B lower if more e^- around atom

$$E = h\nu \sim B_{(actual)} \quad \Rightarrow \text{more } e^-,\ B \downarrow,\ \nu \downarrow$$

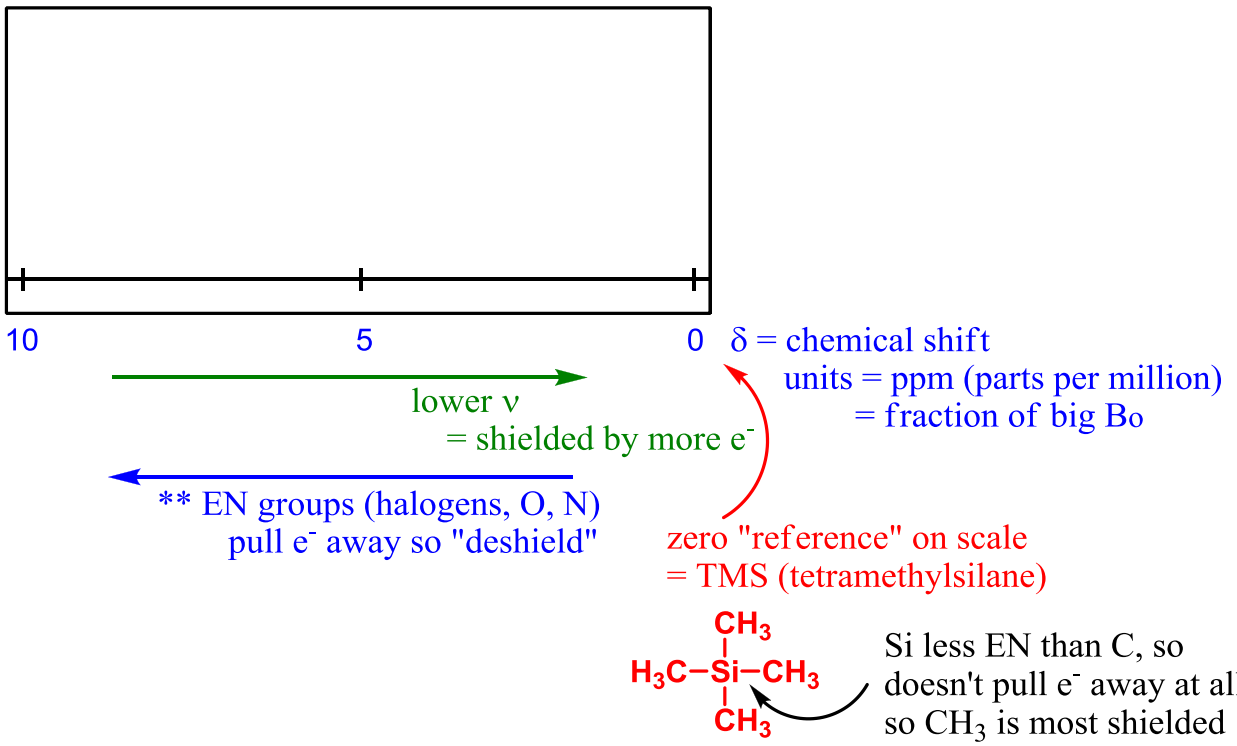


Figure 15.5 (14.5): $(CH_3)_3C\text{-}CH_2\text{-}Br$

closer to Br ∴ higher ν (deshielded)