*CHEM 242 – Lecture 21 05/03/2014*

Overheads: - Outline, NMR Bruice

Recap Monday:

Mass Spectrometry:

* Molecules ionized, see peaks for cations. Taller peak = more molecules with that mass.

Highest mass peak = 72 molecular ion = whole molecule but charged (M+)

Other Peaks: lower mass = fragmentation peaks

M+ extremely high energy, breaks into smaller bits

Tallest Peak = Base Peak

= most stable cation (can be M+ or fragment)

= set to 100%, everything else is relative to it



Infrared (IR) Spectroscopy

* Vibration of bonds



Downward peaks in spectrum mean less light passing through

* Position depends on: - atoms in bond

- strength of bond

Hooke’s law: (for spring)

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

= reduced mass = M1M2

M1+M2

🡩 if M 🡩  🡫 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 (RCO2H: 3300-2500, extremely broad)

14.25 amine (N-H or NH2): 3500-3300, medium

→ less broad than OH (less H-bonding)

→ 2 peaks if NH2

Table 14.4/13.4 gives IR frequencies

NMR Spectroscopy



Nuclei of some atoms (including 1H) have “spin”



Key Point: electrons also tiny magnets (moving – charge)

→ line up opposite to Bo

→ come between nucleus and BIG Bo

electrons “shield” nucleus from Bo, so actual B lower if more e– around atom

E = h ~ B(actual) more e– , B ↓ ,  ↓

Figure 15.5 (14.5): (CH3)3C-CH2-Br

closer to Br higher  (deshielded)