

Today

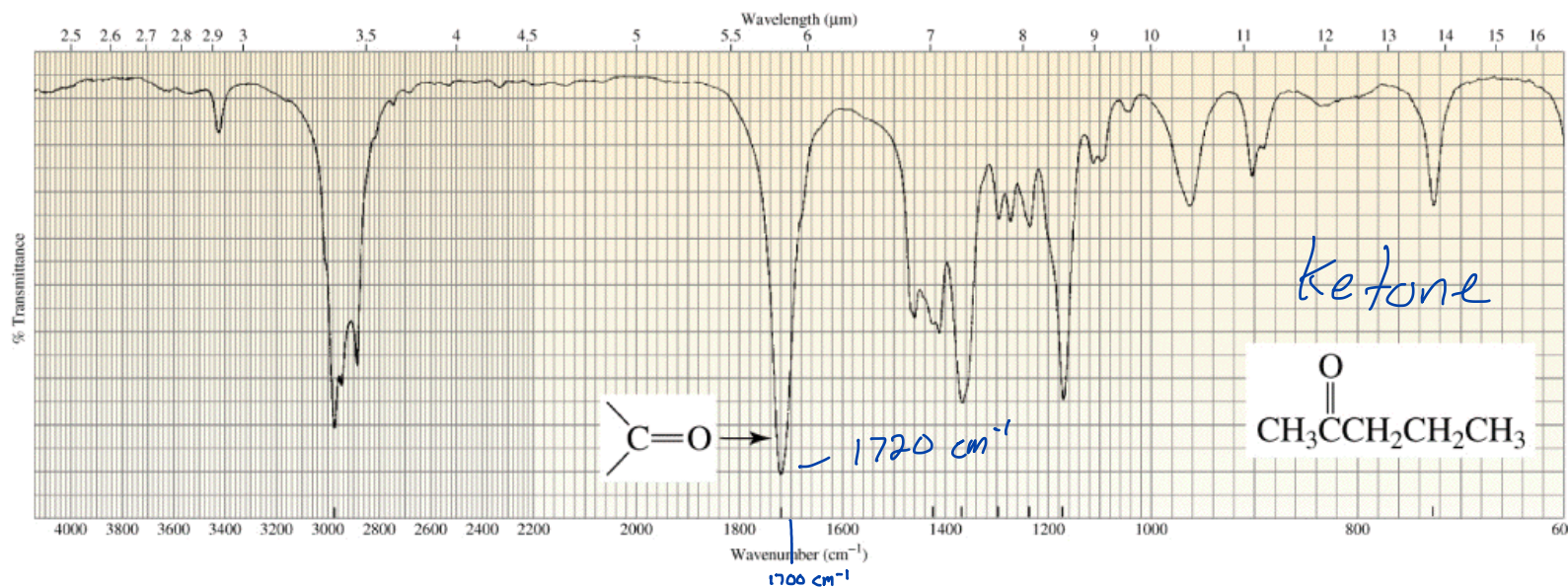
Finish Infrared Spectroscopy (for now)
Section 13.10 - 13.18

Start NMR Spectroscopy
Chap 14

Next Class

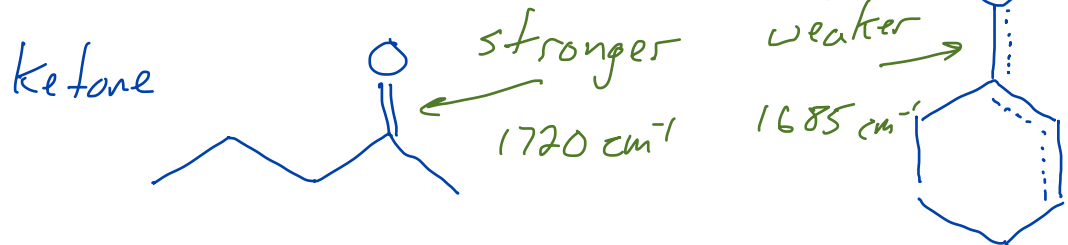
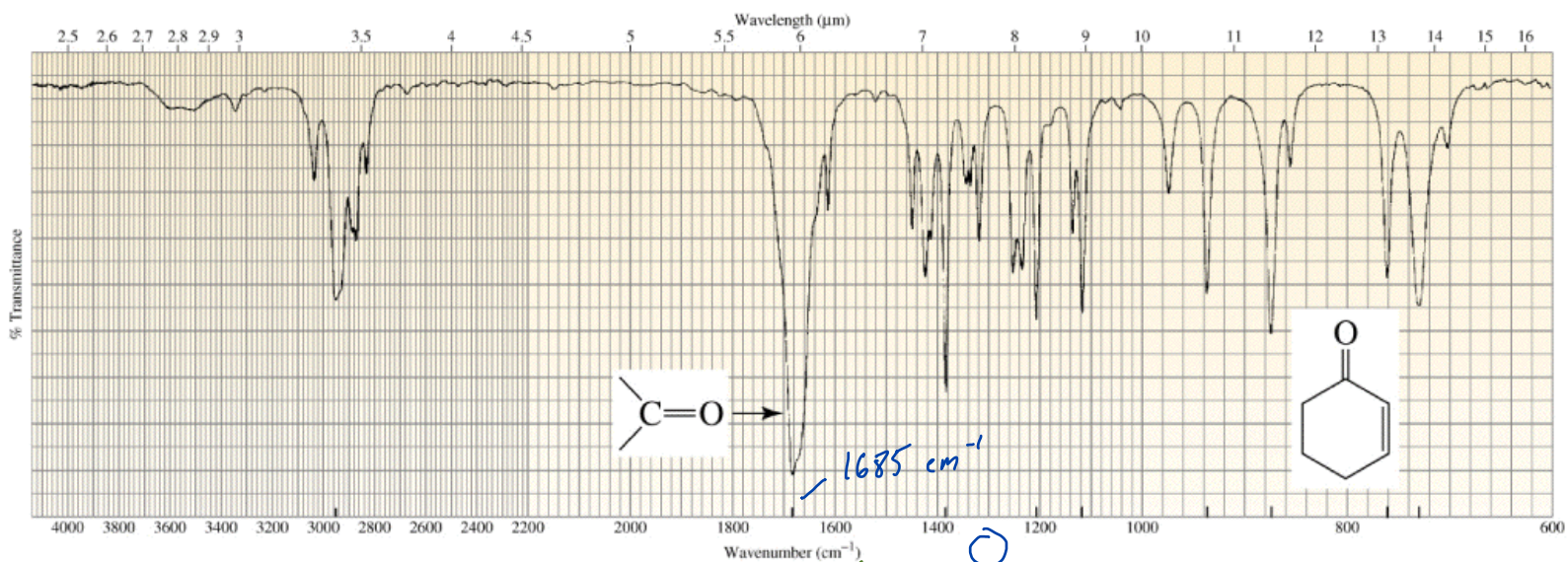
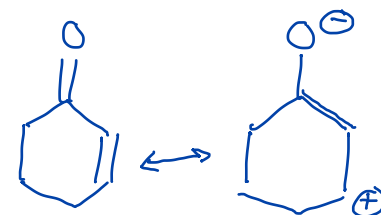
Start NMR Spectroscopy
Chap 14

Fine Tuning Position, C=O's carbonyl functional group



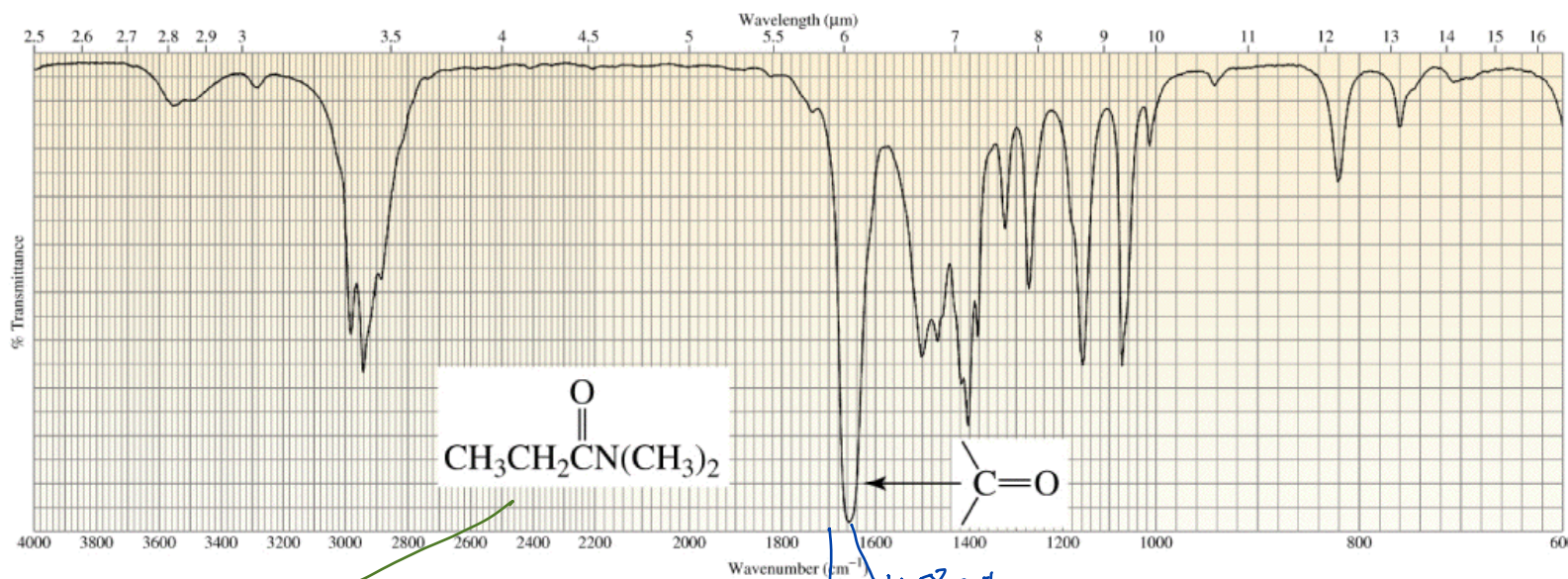
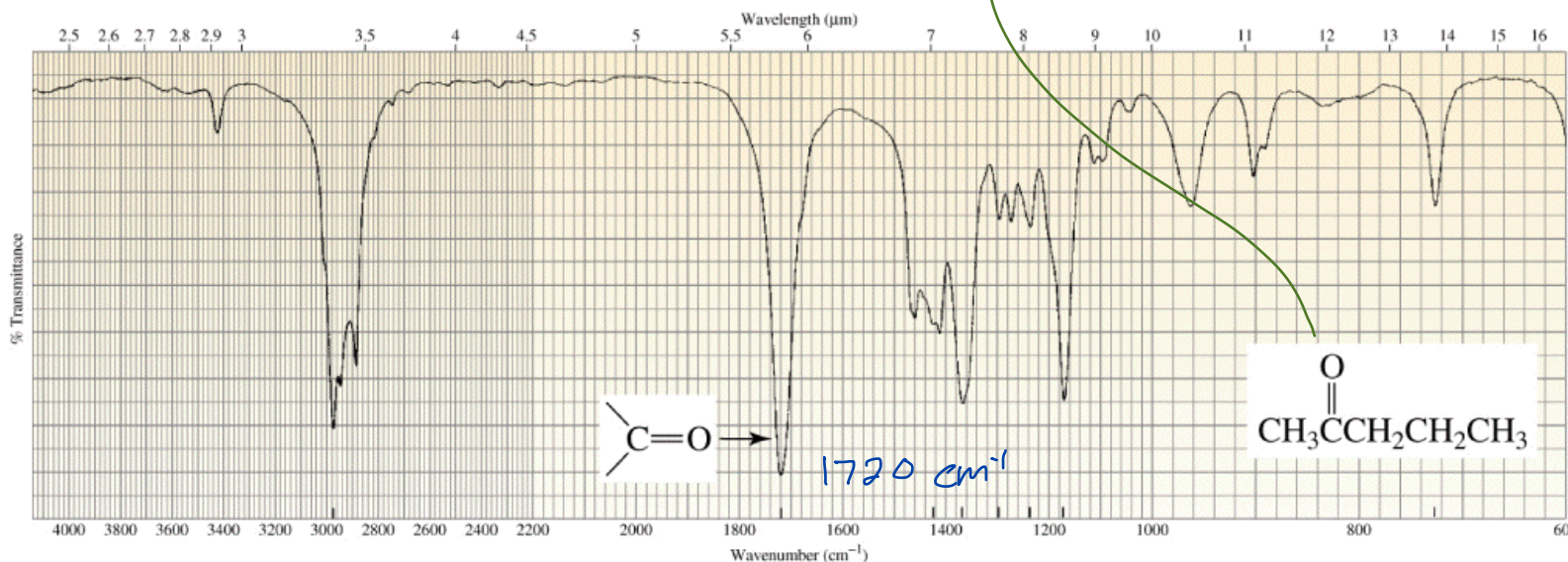
C=O peak moves based on what is next to the C=O

3 or more p orbitals in a row the e^- in those orbitals will be delocalized



α - β unsaturated ketone ketone adjacent to a db

Fine Tuning Position, C=O's

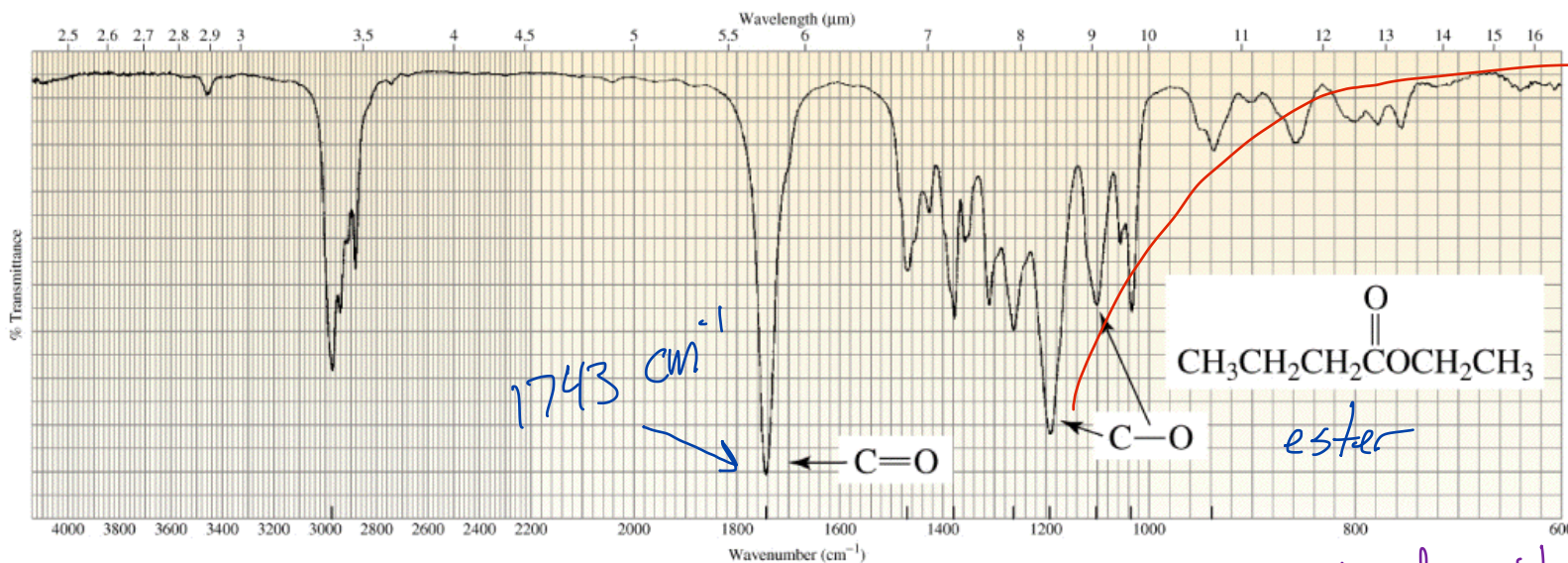
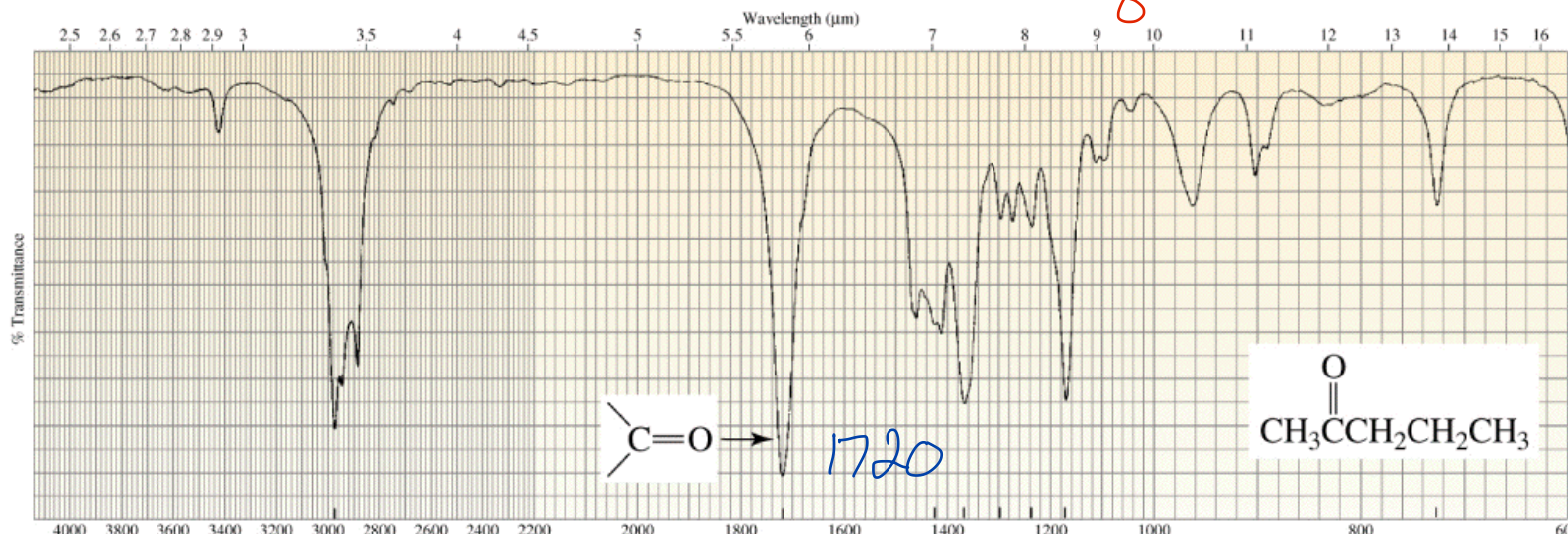


e⁻ delocalization causes C=O to be a little weaker in an amide as compared to a ketone so amides appear lower than 1700 cm⁻¹

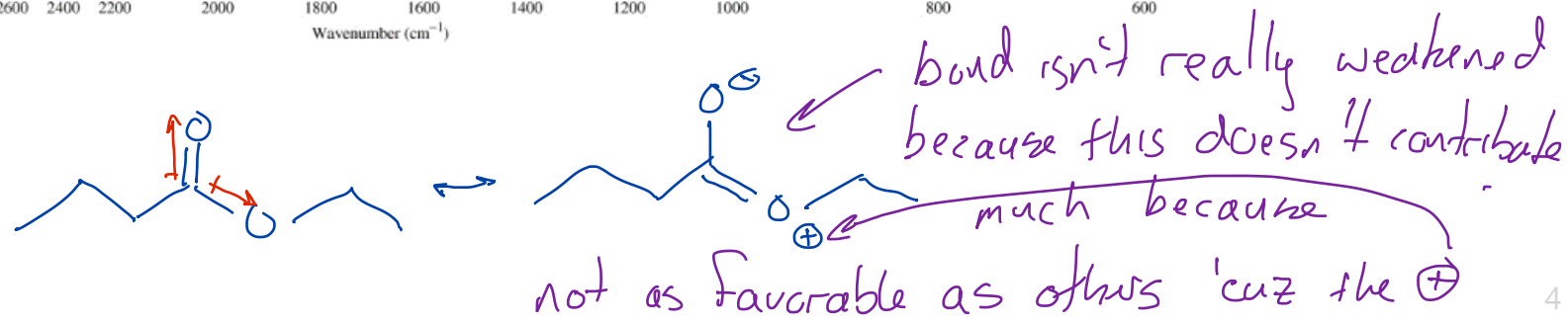
amide
amide linkage is a peptide bond



Fine Tuning Position, C=O's



for esters
is higher
than for
ethers

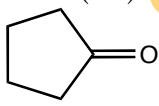


IR Interpretation Guide

Additional information for analyzing C=O stretches:

aldehyde: $\text{RC}(=\text{O})\text{H}$ 1730, $\text{R=CHC}(=\text{O})\text{H}$ 1705

unstrained ketone: $\text{RC}(=\text{O})\text{R}$ 1715, $\text{R=CHC}(=\text{O})\text{R}$ 1690

strained ketone:  1750

ester: $\text{RC}(=\text{O})\text{OR}$ 1735, $\text{R=CHC}(=\text{O})\text{OR}$ 1715.

amide: $\text{R}(\text{C}=\text{O})\text{NH}_2$ < 1700

acid: 1710 usually broad for a C=O

Additional information for analyzing C-H stretches:

If sp^3 C-H stretch at $< 3000 \text{ cm}^{-1}$ then look around 1400, sp^3 C-H bend is at 1430 and if peak at 1380 also present then sp^3 C-H is CH_3 .

If sp^2 C-H stretch at $> 3000 \text{ cm}^{-1}$, and not benzene gives rise to bending vibrations from 1000–600.

Some abbreviations for vibrational modes

ν stretching

δ in-plane bending or deformation

ρ_w wagging

ρ_r rocking

ρ_t twisting

π out-of-plane bending

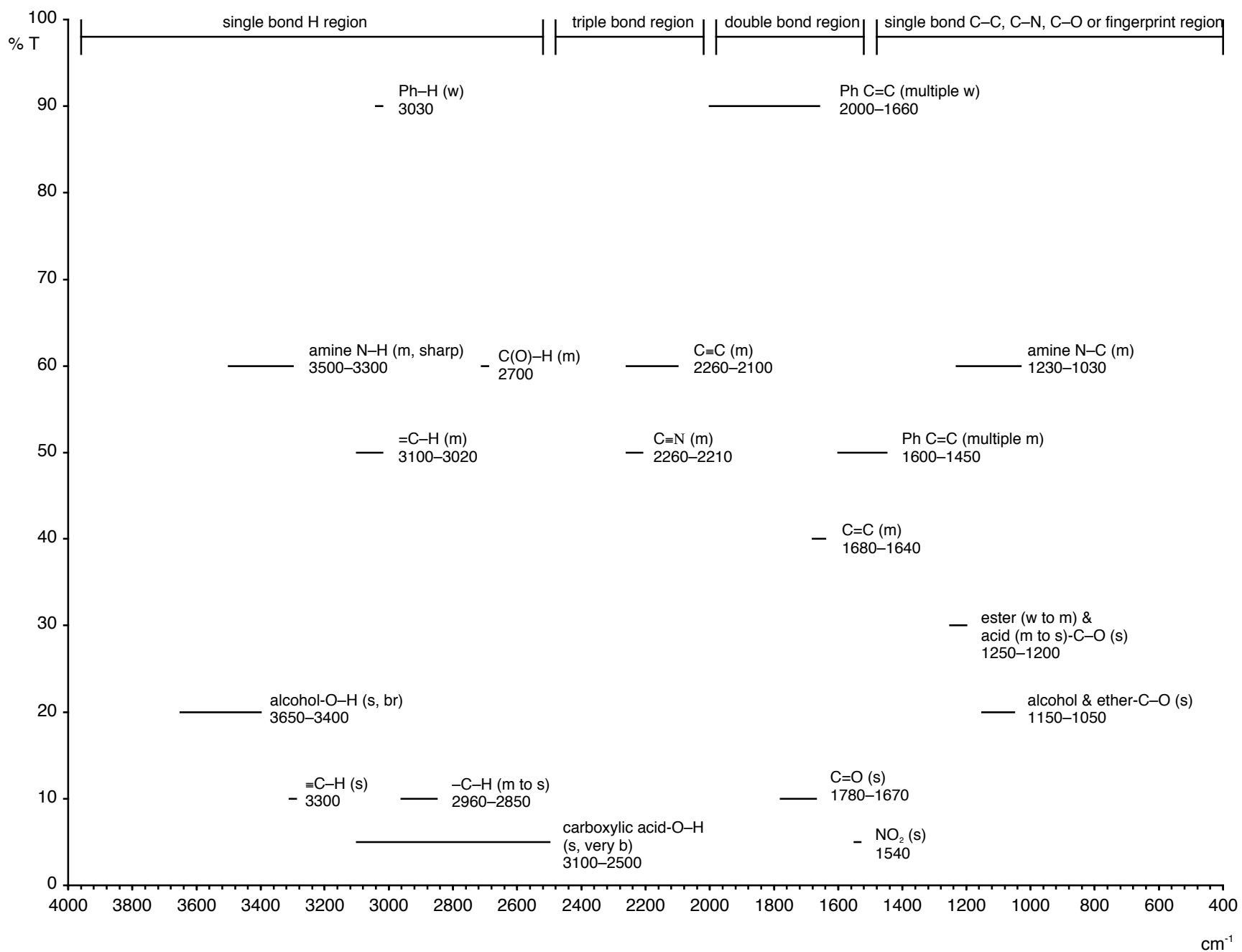
Abbreviations used to further characterize vibration modes

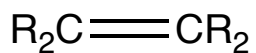
a antisymmetric

s symmetric

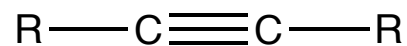
d degenerate

For example, references to $\nu_s(\text{C}-\text{Cl})$ are references to the symmetrical stretching mode of a C to Cl bond.

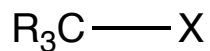




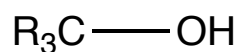
alkenes



alkynes



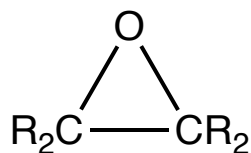
X = Cl, Br, I
Alkyl Halides



alcohols

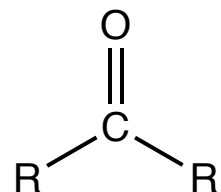


ethers

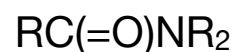


epoxides

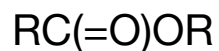
and more...



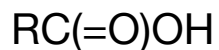
ketones (R, R' ≠ H) and
aldehydes (R or R' = H)



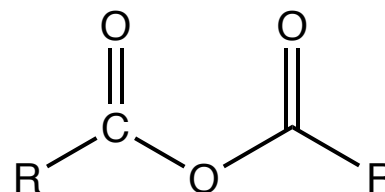
amides



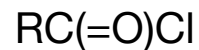
esters (R ≠ H)



carboxylic acids



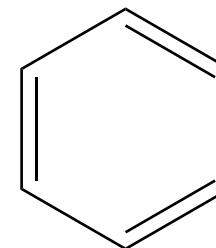
anhydrides



acid chlorides



nitriles



aromatics

and more...

Strategies for using IR spectroscopy to identify functional groups.

Examine formula and look for possible functional groups in IR spectrum

Closely examine positions of C–H peaks for additional information

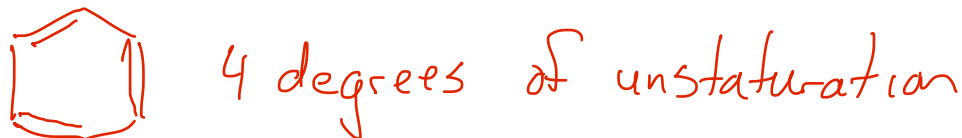
sp^2 vs sp^3 C atoms

presence or absence of CH_3 groups

Position of C=O peaks

ketone vs aldehyde vs ester vs carboxylic acid

Rule benzene rings in or out using degree of unsaturation ($2n+2$ rule)



Examine IR spectrum for obvious functional groups

Double check consistency: for example

do not claim a C=O peak is an ester if the molecule has only 1 O atom

do not claim nitrile if there are no N atoms