Today

Infrared Spectroscopy

Next Class

Chapter 21.1 – 21.3

Second Class from Today

Chapter 21.4 – 21.7

Third Class from Today

Chapter 21.8 – 21.9 , Chemistry Matters

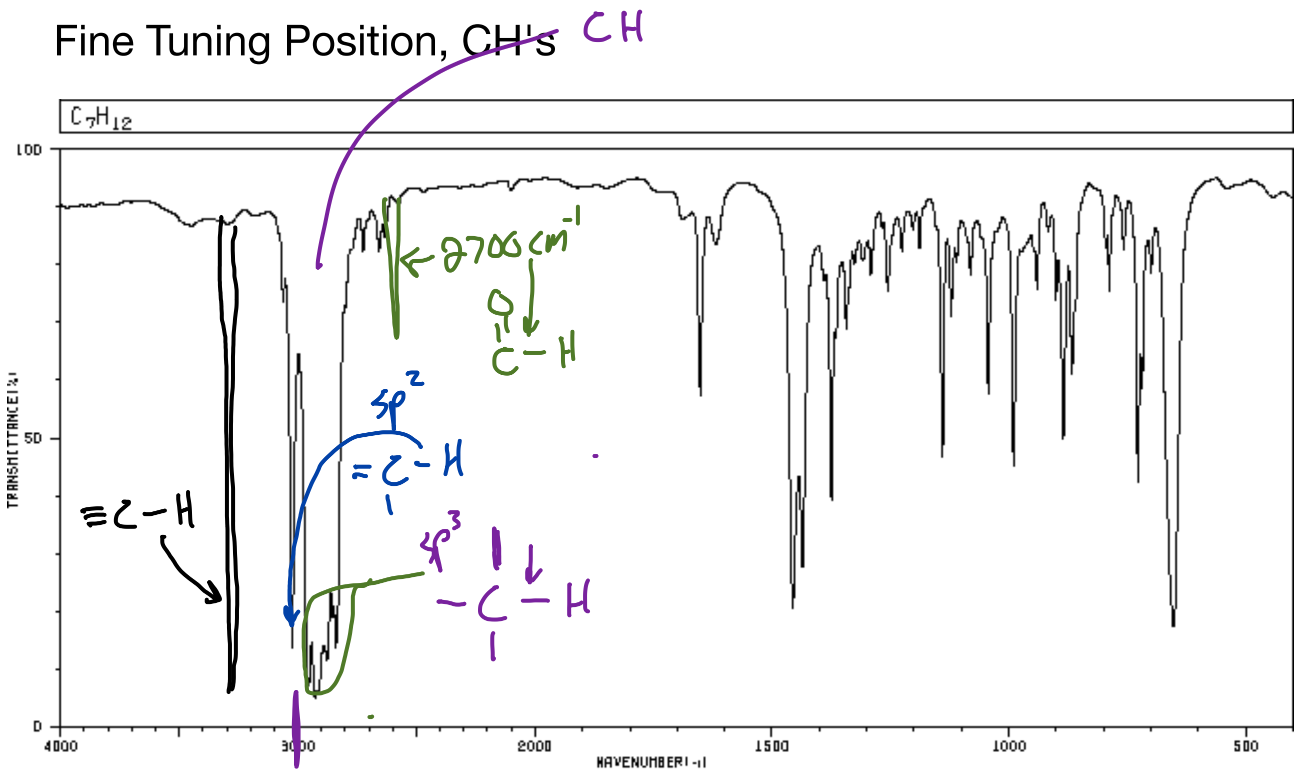
Monday office hours rescheduled to 1:10 to 2:10 from now on.

Please rework, on a separate piece of paper, test 1 and hand in on ~~Wednesday, March 19~~ Monday, March 24.

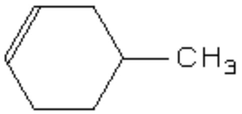
Rework means for each question that your did not receive full credit provide a more complete answer.

I do not need your test back, please just hand in the reworked answers.

Fine Tuning Position, CH's



3063	70	2839	13	1344	66	1122	68	886	47
3025	13	1651	55	1326	77	1111	77	867	58
2954	6	1458	20	1309	77	1081	74	789	72
2928	4	1436	26	1292	74	1044	66	728	41
2915	6	1390	74	1256	72	990	43	719	57
2878	10	1375	37	1227	79	941	72	701	74
2862	18	1366	64	1141	44	901	70	663	16



≡C–H 3300 cm⁻¹

=C–H to the left of 3000 cm⁻¹

–C–H to right of 3000 cm⁻¹

$\overset{O}{\|}$
C–H at 2700 cm⁻¹

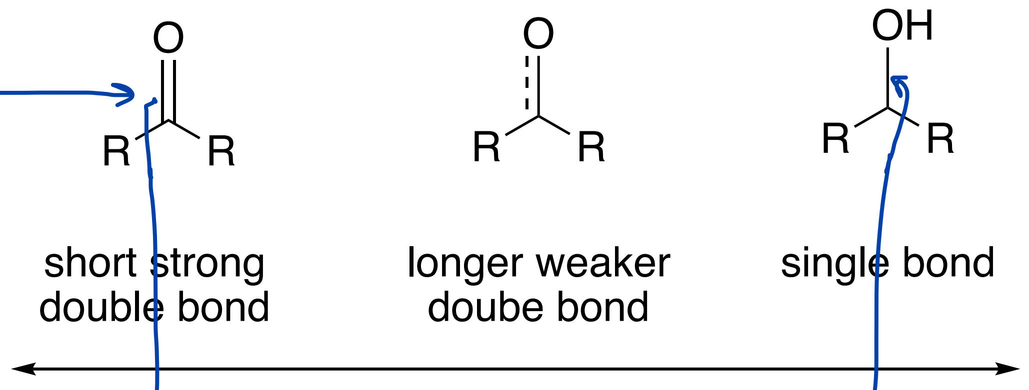
National Institute of Advanced Industrial Science and Technology (AIST), Japan http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi

Fine Tuning Identification of Carbonyl Peaks

$$\bar{\nu} = \frac{1}{2\pi c}\left[\frac{f(m_1 + m_2)}{m_1 m_2}\right]$$

when these stretch the vibration really changes the dipole of the molecule...

Intense... easy to see peaks



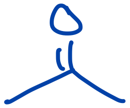
short strong double bond

longer weaker doube bond

single bond

higher wave number

lower wave number



$1715\ cm^{-1}$

strong bond

large f

higher frequency

$\sim 1050\ cm^{-1}$

weaker bond

smaller f

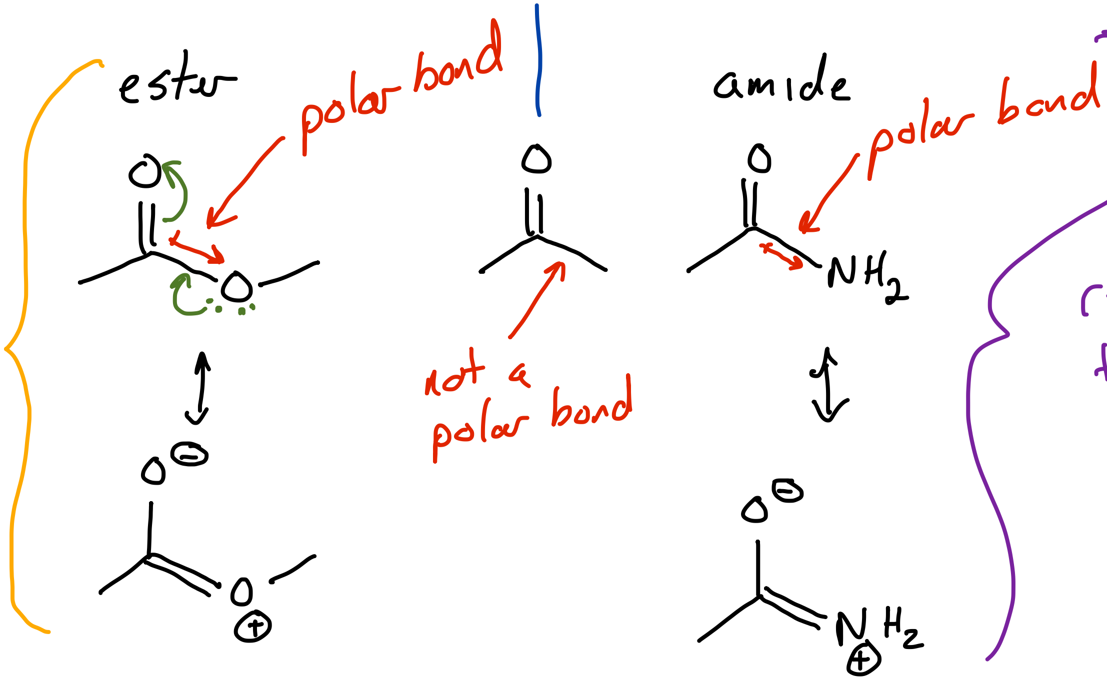
lower frequency

Fine Tuning Position, C=O's

vibrates @ higher freq   1715 cm^{-1} vibrates at lower freq

Resonance vs Electronegativity

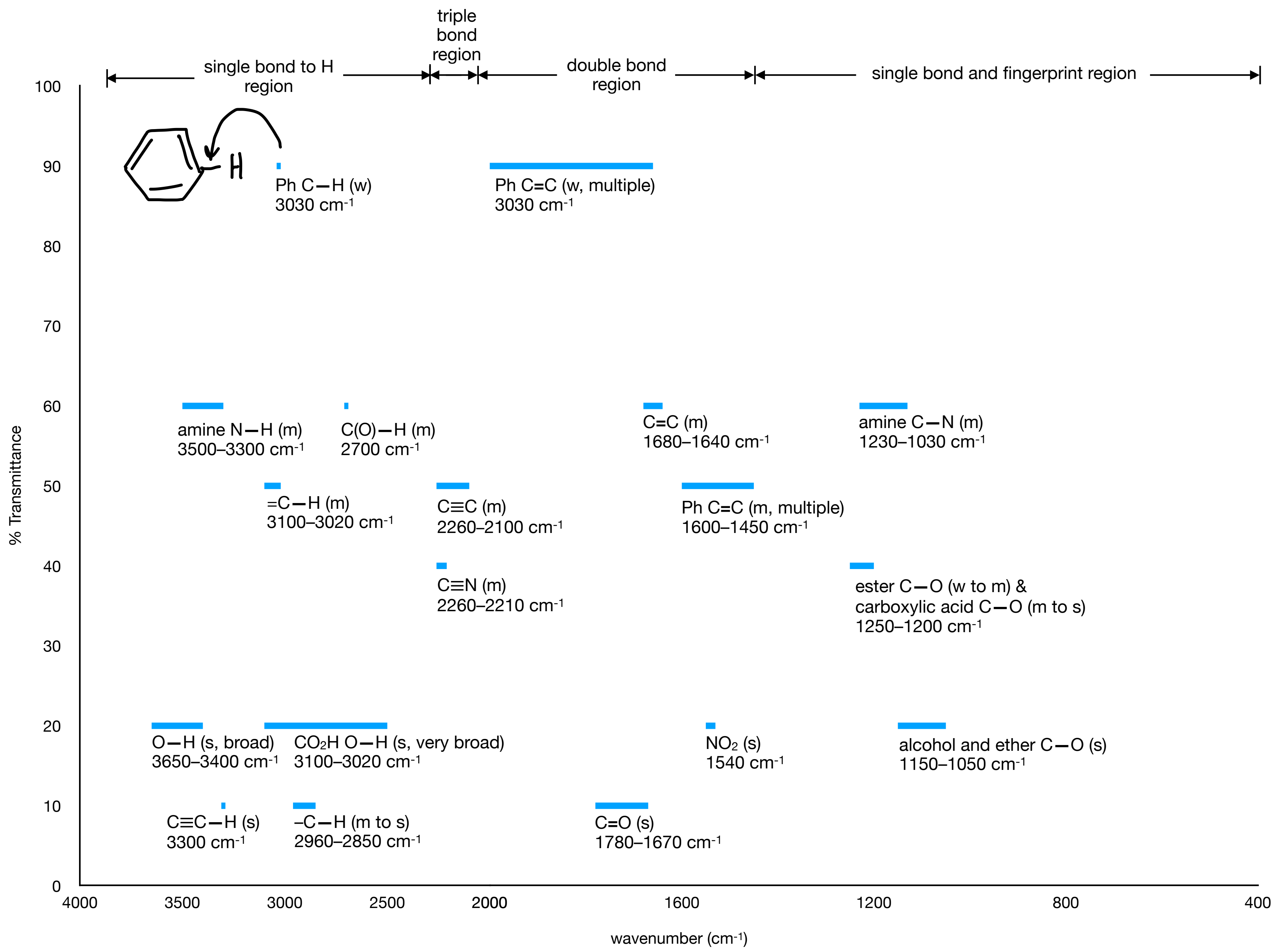
eneg effect wins and the C=O bond is stronger



resonance contribution to bond strength outweighs eneg atom contribution to bond strength the C=O bond is weaker

resonance contributors suggest C=O is more like C--O
suggest bond is weaker
suggest vibration is at lower frequency

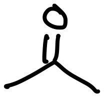
eneg atoms make C of C=O more ⊕ ...
suggests C=O is stronger


single bond to H region
triple bond region
double bond region
single bond and fingerprint region
100
90
80
70
60
50
40
30
20
10
0
% Transmittance
H
Ph C—H (w)
3030 cm^{-1}
Ph C=C (w, multiple)
3030 cm^{-1}
amine N—H (m)
3500–3300 cm^{-1}
C(O)—H (m)
2700 cm^{-1}
C=C (m)
1680–1640 cm^{-1}
amine C—N (m)
1230–1030 cm^{-1}
=C—H (m)
3100–3020 cm^{-1}
C≡C (m)
2260–2100 cm^{-1}
Ph C=C (m, multiple)
1600–1450 cm^{-1}
C≡N (m)
2260–2210 cm^{-1}
ester C—O (w to m) &
carboxylic acid C—O (m to s)
1250–1200 cm^{-1}
O—H (s, broad)
3650–3400 cm^{-1}
CO$_2$H O—H (s, very broad)
3100–3020 cm^{-1}
NO$_2$ (s)
1540 cm^{-1}
alcohol and ether C—O (s)
1150–1050 cm^{-1}
C≡C—H (s)
3300 cm^{-1}
–C—H (m to s)
2960–2850 cm^{-1}
C=O (s)
1780–1670 cm^{-1}
4000
3500
3000
2500
2000
1600
1200
800
400
wavenumber (cm^{-1})

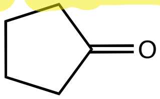
IR Interpretation Guide

Additional information for analyzing C=O stretches:

aldehyde: RC(=O)H 1730, R=CHC(=O)H 1705
unstrained ketone: RC(=O)R 1715, R=CHC(=O)R 1690



$1715\ cm^{-1}$

strained ketone:  1750

ester: RC(=O)OR 1735, R=CHC(=O)OR 1715.

amide: R(C=O)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 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 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 ν_s(C–Cl) are references to the symmetrical stretching mode of a C to Cl bond.

Strategies for using IR spectroscopy to identify functional groups.

Examine formula and look for possible functional groups in IR spectrum
- use 2n+2 rule to rule π bonds in or out
- 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
  - amide vs 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 for 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
- look for confirmation in assignments:
  - aldehyde, find both C=O and C(O)-H peaks
  - ester C=O and C(O)-O-R peaks