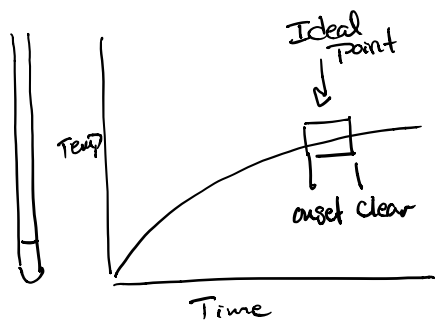


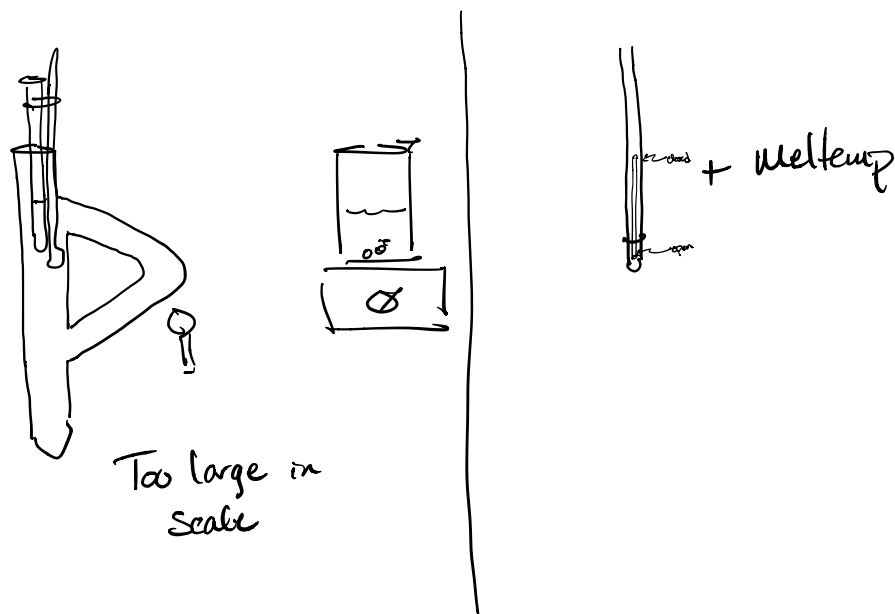
Lab #8 Boiling Point & FTIR

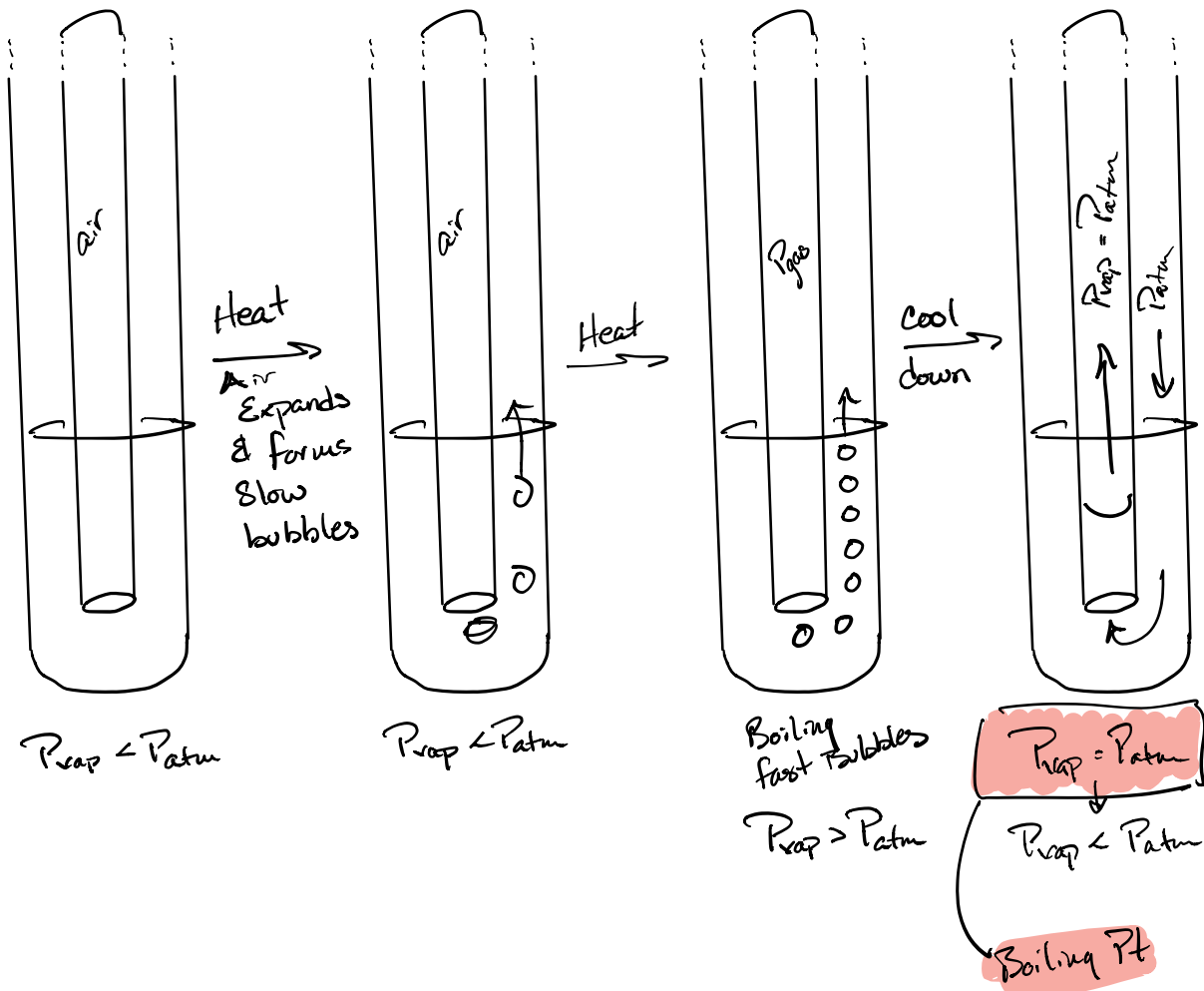
Boiling Point



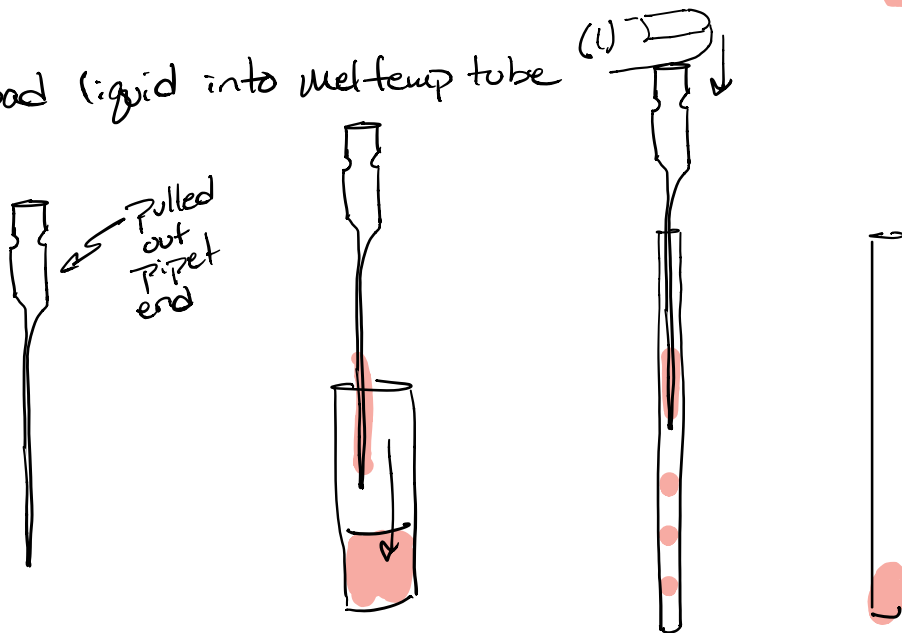
Boiling point = $P_{\text{vap}} = P_{\text{atm}}$
Sharp point

MP Range (onset - clear point)

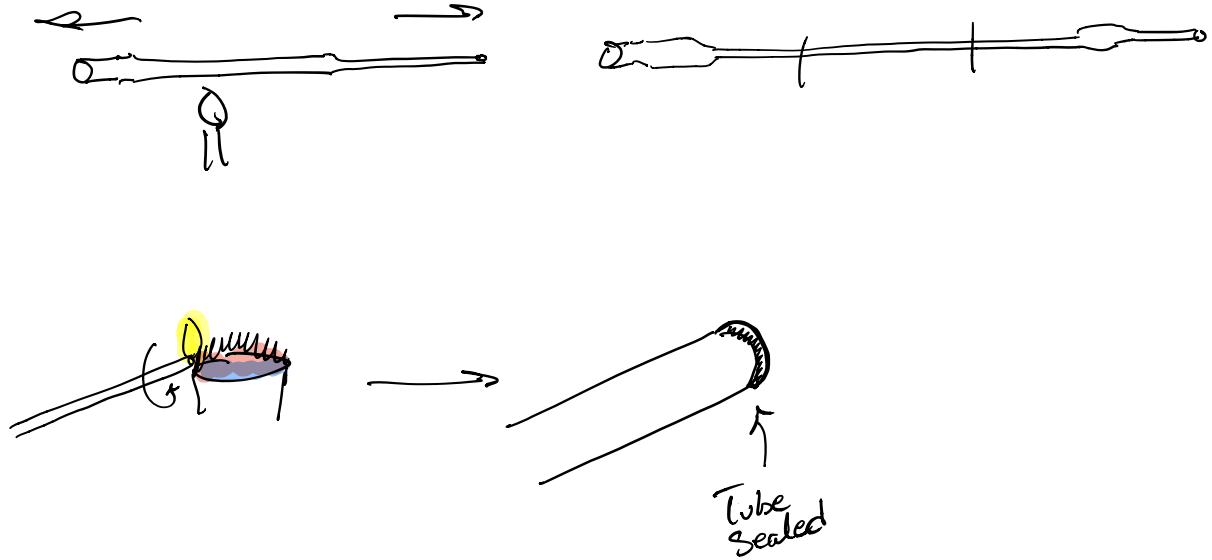




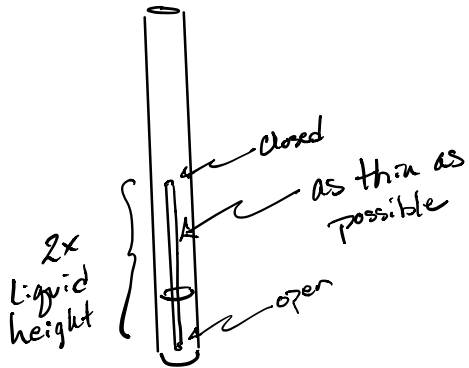
① Load liquid into meltemp tube

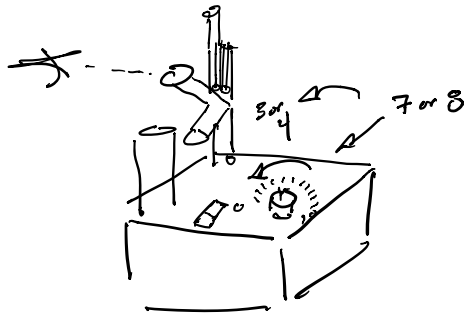
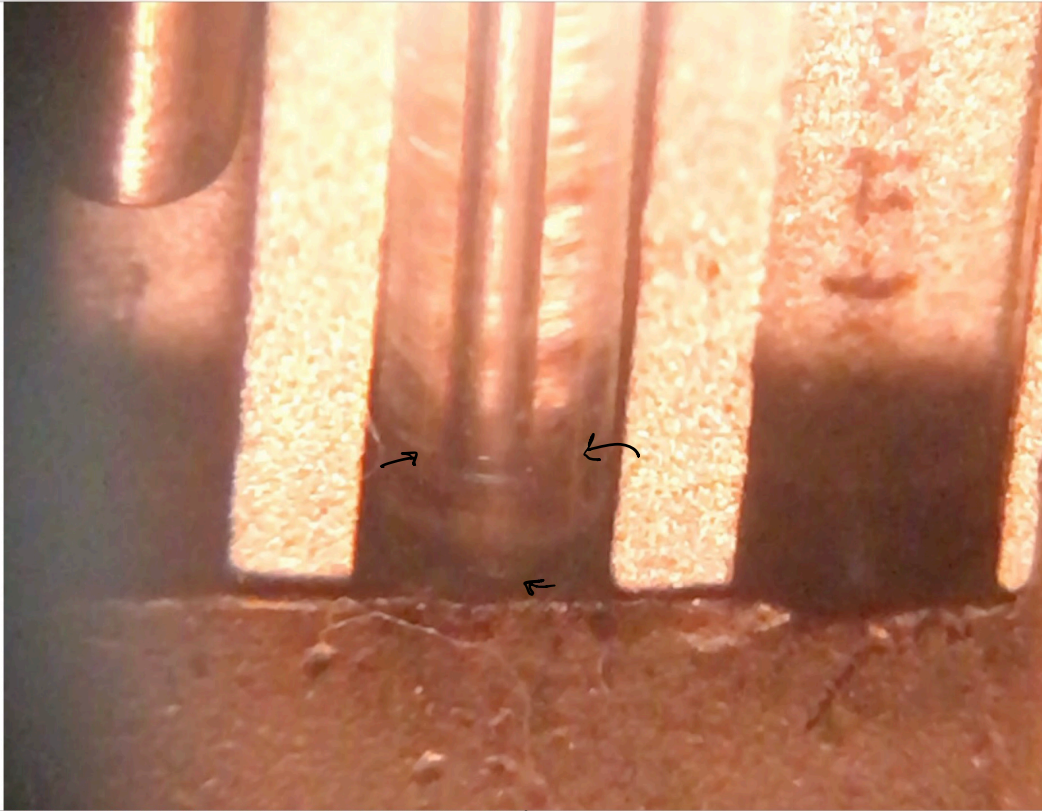


② Make the dumbbell

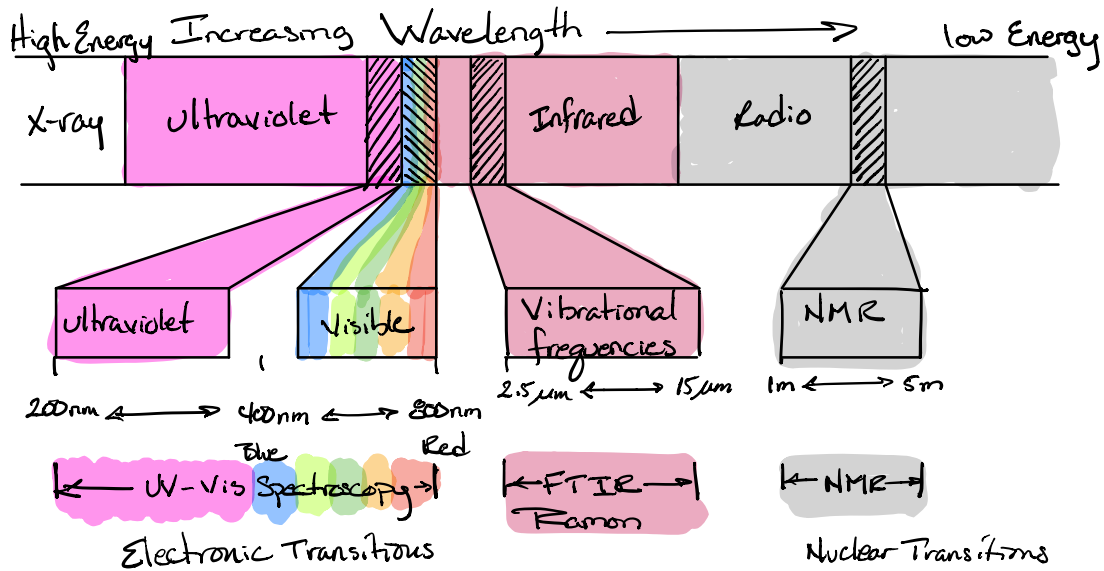


③ Load dumbbell





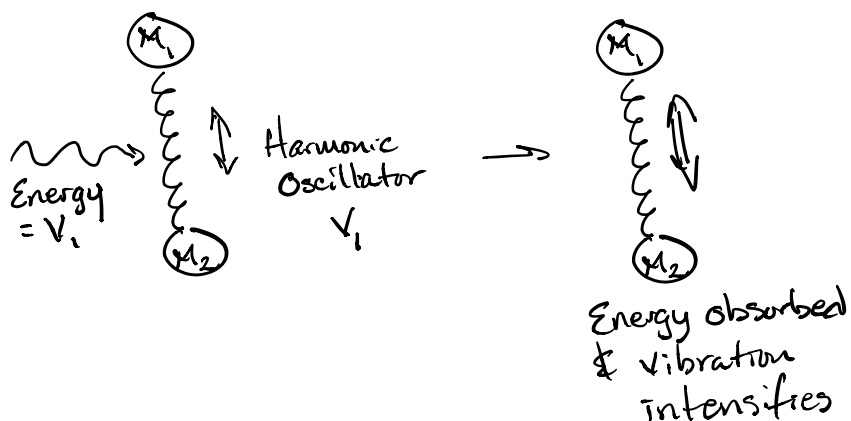
Infrared Spectroscopy (IR or sometime FTIR)



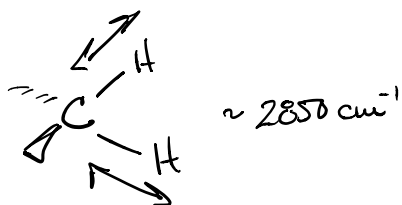
Wavelength = $\mu\text{m} = 1 \times 10^{-6} \text{ m}$

Wavenumber = $\text{cm}^{-1} = \frac{1}{\mu\text{m}} \times \frac{10,000 \mu\text{m}}{1 \text{ cm}} = \frac{1}{\mu\text{m}} \times 10,000$

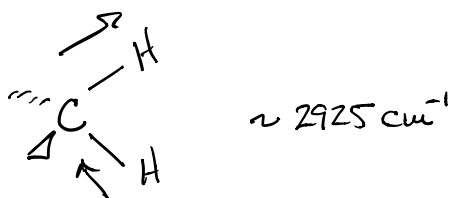
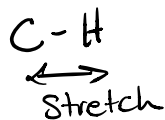
Vibrational frequencies



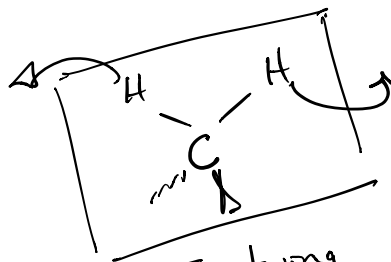
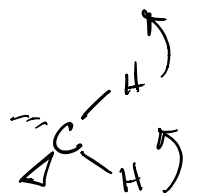
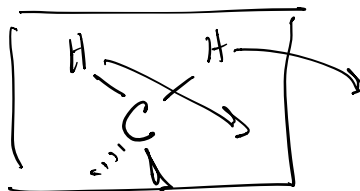
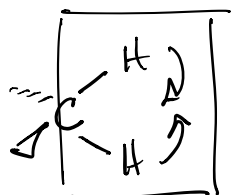
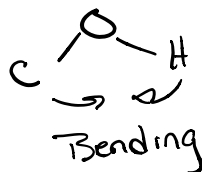
Simple vibrational frequencies

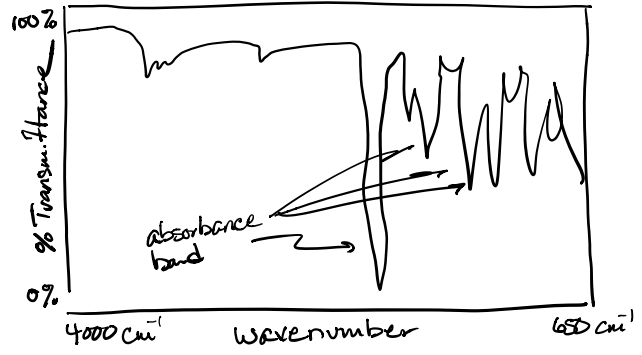
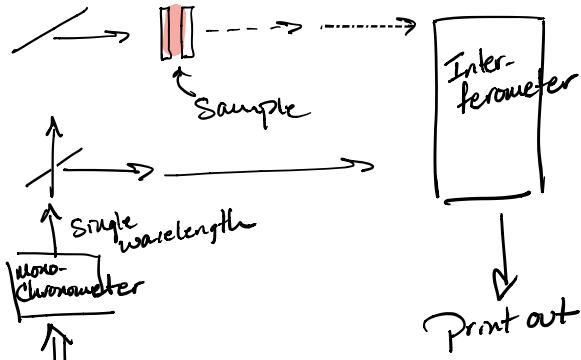


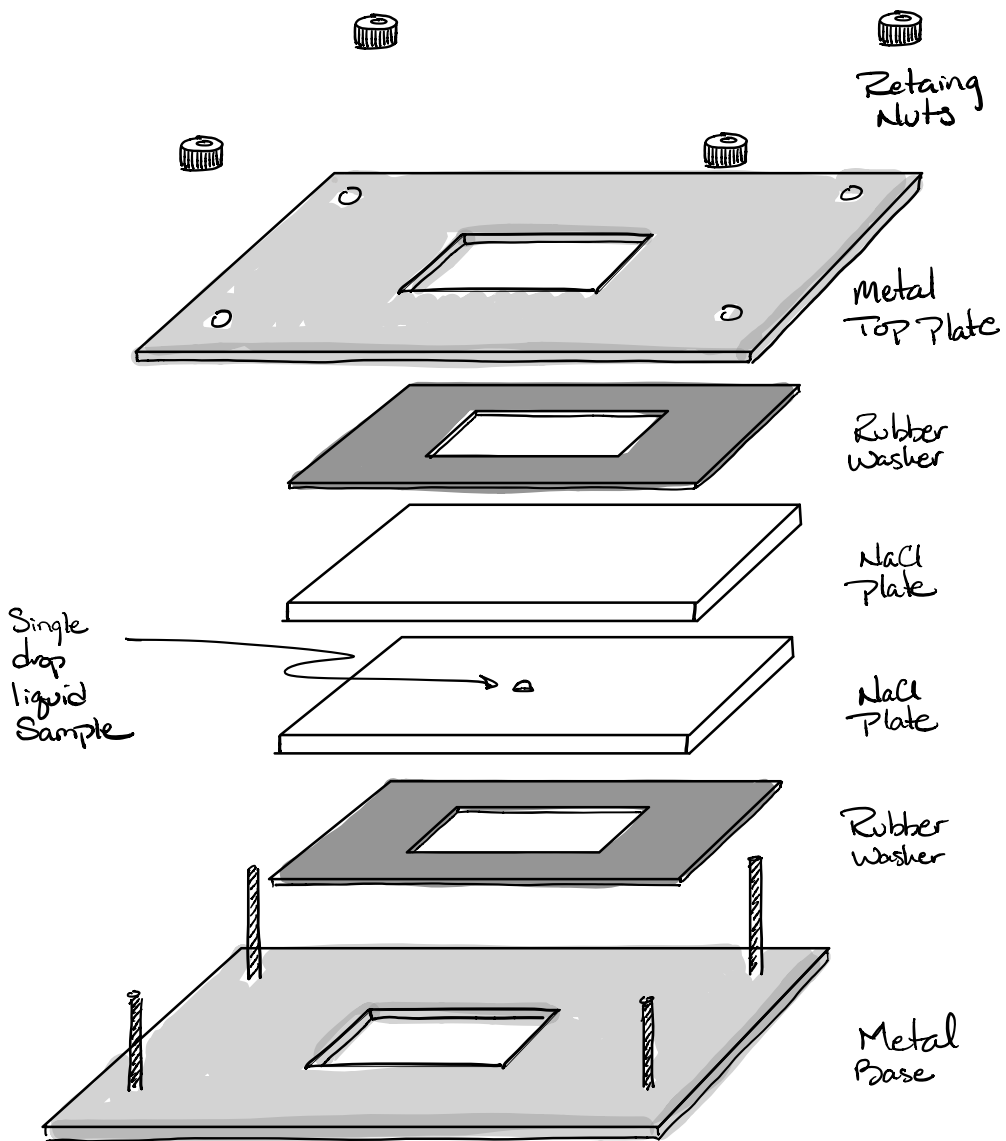
Symmetric Stretch

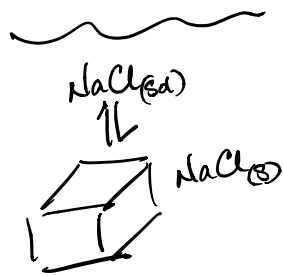
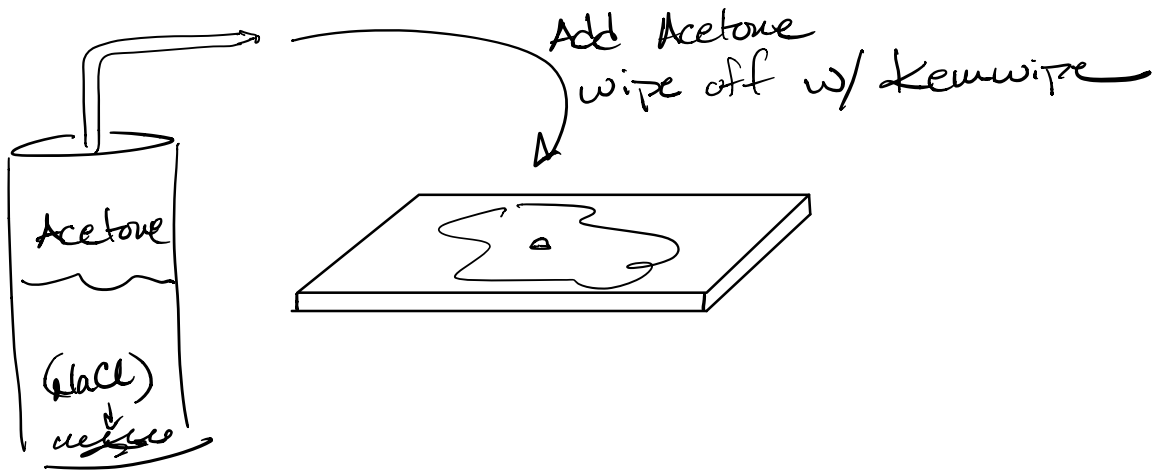


Asymmetric Stretch









OBSERVATION
PUDDLES AND WORMS...
IT MUST HAVE RAINED.
INFERENCE
AN IR BAND OF THIS SIZE AND SHAPE...
INFERENCE
PROBABLY THAT FUNCTIONAL GROUP.

ALL IR BANDS ARE EQUAL, BUT SOME ARE MORE EQUAL THAN OTHERS.

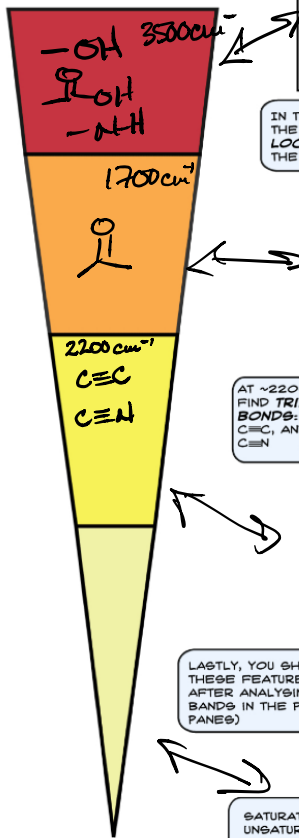
Alkyne (stretch)	ca. 3300	1x
Aldehyde	2900-2800	1.4x
	2800-2700	1.5x
Alkane	not interpretatively useful	
Alkene	1600-1600	1.9x
Aromatic	1600 and 1475	6.2x
Alkyne	2250-2100	4.6x
Aldehyde	1740-1720	5.7x
Ketone	1725-1705	5.8x
Carboxylic Acid	1725-1700	5.8x
Ester	1750-1730	5.7x
Amide	1670-1640	6.0x
Anhydride	1810 and 1760	5.5x
Acid Chloride	1800	5.5x
Alcohol, Ethers, Esters, Carboxylic Acids, Anhydrides	1300-1000	7.6x

MOVING DOWN THE CHART ONE AT A TIME, MATCHING BANDS AS YOU GO, IS NOT A USEFUL STRATEGY.

INSTEAD, LET'S ARRANGE THEM BY THEIR INTERPRETIVE POWER.

Alkyne (stretch)	ca. 3300
Aldehyde	2900-2800
	2800-2700
Alkene	1600-1600
Aromatic	1600 and 1475
Alkyne	2250-2100
Aldehyde	1740-1720
Ketone	1725-1705
Carboxylic Acid	1725-1700
Ester	1750-1730
Amide	1670-1640
Anhydride	1810 and 1760
Alcohol, Ethers, Esters, Carboxylic Acids, Anhydrides	1300-1000
Alkane	not interpretatively useful

GREAT INTERPRETIVE POWER



THIS IS THE FIRST REGION YOU SHOULD LOOK AT, AND THERE ARE 4 DIFFERENT SHAPES OF BANDS THAT YOU MAY SEE HERE.

...AND IF YOU DON'T SEE ANY BAND HERE, YOU MOST LIKELY DON'T HAVE ANY OF THESE FUNCTIONAL GROUPS (FG)

A SMOOTH TONGUE MEANS AN ALCOHOL. -OH

VAMPIRE FANGS MEANS A PRIMARY AMINE... -NH2

ONE KNOCK-OUT FANG MEANS A 2° AMINE OR A TERMINAL ALKYNE. -NH- -C#H

HAIRY BEARD IS A SIGN FOR A CARBOXYLIC ACID. -COOH

Smooth intense
Weak sharp
Weak single
Sawtooth strong

IN THE C=O REGION, IT'S NOT THE SHAPE, BUT THE EXACT LOCATION THAT REVEALS THE IDENTITY OF THE FG.

NOTE THAT THE EXACT POSITION DEPENDS ON THE SURROUNDING ENVIRONMENT:

STRAIN, OR CONJUGATED AT C=C +30CM⁻¹

CONJUGATED AT C=O -30CM⁻¹

ACID CHLORIDES	1810
ANHYDRIDES	1820
ETHERS	1760
ALDEHYDES	1735
KETONES	1715
ACIDS	1710
AMIDES	1660

AT ~2200 CM⁻¹, WE FIND TRIPLE BONDS: C≡C, AND C≡N

USUALLY SHARP (CAN BE SMALLISH)

HINT: USE 3300 CM⁻¹ TO DISTINGUISH TERMINAL AND INTERNAL ALKYNES.

Interpreting IR spectra

JON - JKWCHUI@UVC.CA

LASTLY, YOU SHOULD LOOK AT THESE FEATURES (BUT ONLY AFTER ANALYSING THE MAJOR BANDS IN THE PREVIOUS PAGES)

UNSATURATED C-H STRETCH

SATURATED C-H STRETCH

SATURATED AND UNSATURATED C-H CAN BE PRESENT AT THE SAME TIME.

ALKENE/AROMATIC SUBSTITUTION PATTERN CAN BE SEEN IN THE C-H BEND REGIONS.

MONO: 700-600 cm⁻¹

ORTHO: 750 cm⁻¹

META: 830, 750, 690 cm⁻¹

PARA: 830 cm⁻¹

STRETCHES: 910 (STRONG), 960 (STRONG), 1000 (WEAK), 1070 (STRONG)

MONO: GEM (1,1-) DI-SUBSTITUTED

CIS- TRANS-

LASTLY, A PEAK AT 2700 CM⁻¹, TOGETHER WITH A C=O, IS INDICATIVE OF AN ALDEHYDE.

C-H STRETCH

C=O STRETCH

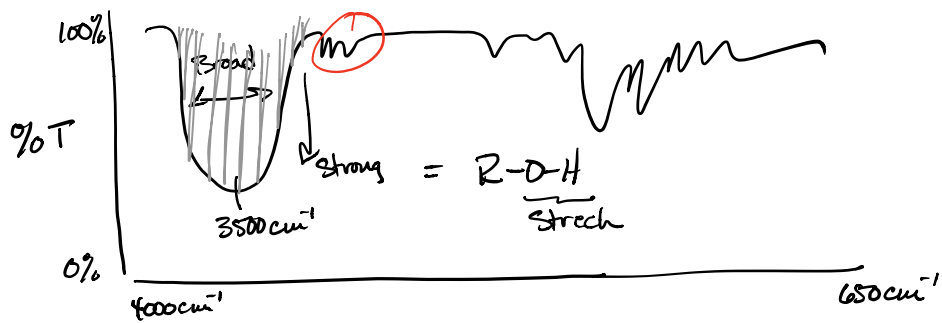
KETONES HAVE NO C-H IN THEM AND CAN HAVE NO 2700 C-H STRETCH PEAKS.

NOTES

** IF YOU'RE NOT SURE WHAT THE DIFFERENCE BETWEEN AN ACID AND AN ALCOHOL IS, DO THE QUICK "FUNCTIONAL GROUP IDENTIFICATION" EXERCISE.

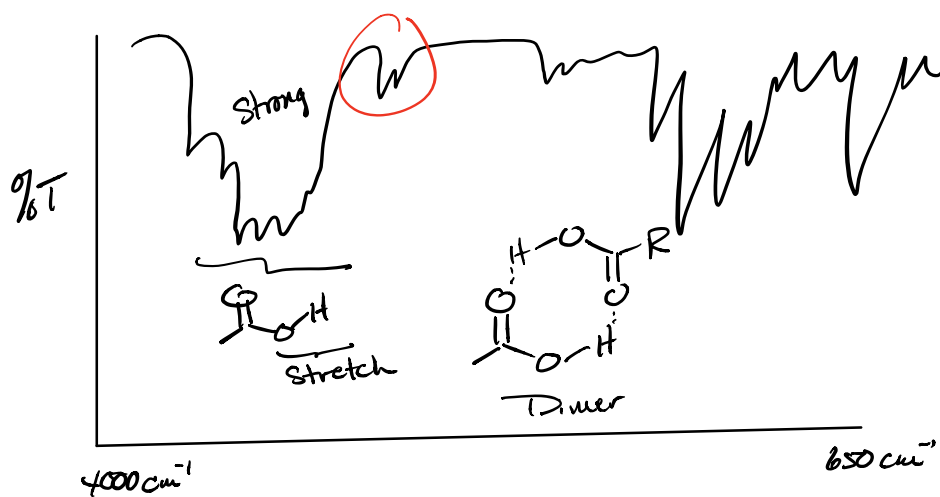
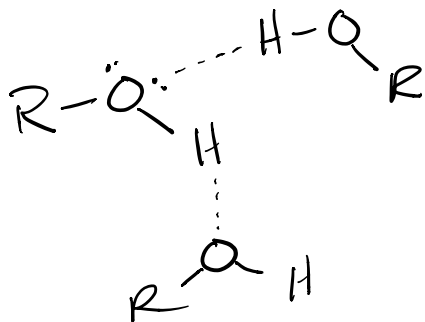
** ...IF YOU HAVE ONE FG, TWO 2° AMINE WOULD LOOK LIKE A 1 AMINE.

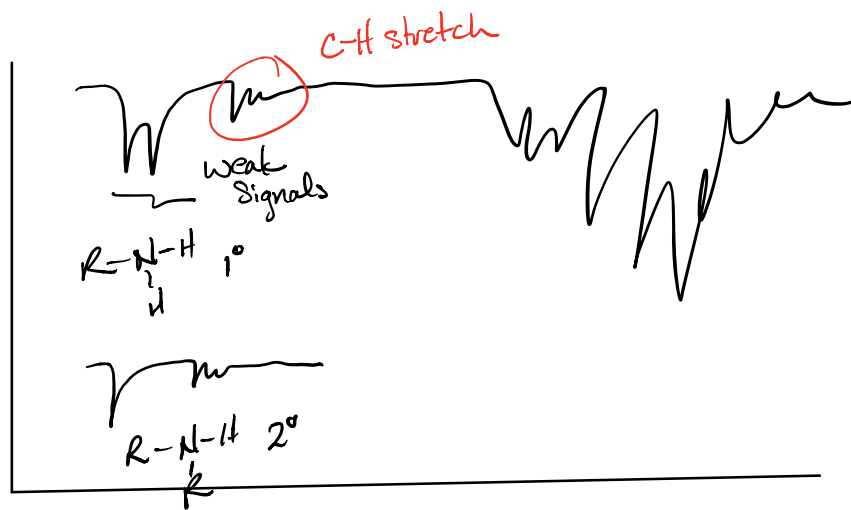
WE LOOKED AT THESE LAST BECAUSE THEY CAN BE AMBIGUOUS TO INTERPRET, OR THEY HAVE ONLY A NARROW NICHE OF USEFULNESS.



Strong 0-20%T
 med 20-70%T
 weak 70%-100%T

Broad Sharp





1700 cm^{-1} Carbonyl Group

