Learning Guide for Chapter 3 - Infrared Spectroscopy

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III. Identifying functional groups - p 6
IV. Interpreting an IR spectrum - p 12

I. Introduction to spectroscopy

Characterizing compounds

What does it mean to characterize a compound?

What are some examples of when you would need to do this?

What are some physical properties of organic compounds, and how can they be used in characterization?

How are chemical tests used to characterize organic compounds?

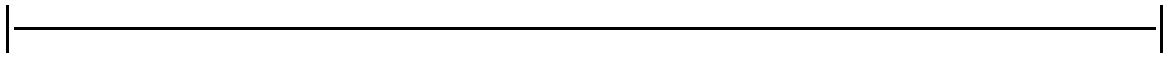
What does spectroscopy use to characterize a compound?

What are the most common kinds of spectroscopy used in organic chemistry, and what kinds of information do they give?

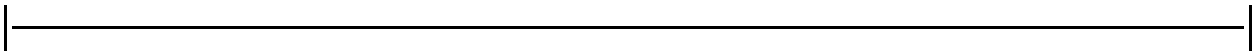
The Electromagnetic Spectrum

What kinds of light are present in the electromagnetic spectrum? How do they affect atoms and molecules?

high energy low energy

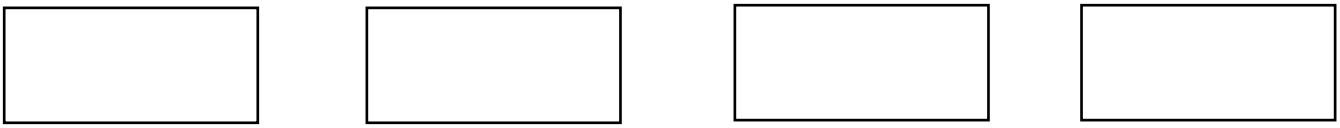


What unit of frequency is used in IR spectroscopy? What is the range of frequencies used in IR spectroscopy?



The IR Spectrometer and and IR Spectrum

What are the essential components of an IR spectrometer?



What is FTIR?

How can you take the IR of a liquid compound?

How can you take an IR of a solid compound?

What does an IR spectrum look like?

II. Molecular vibrations

Types of vibrations

Why do molecules absorb infrared light?

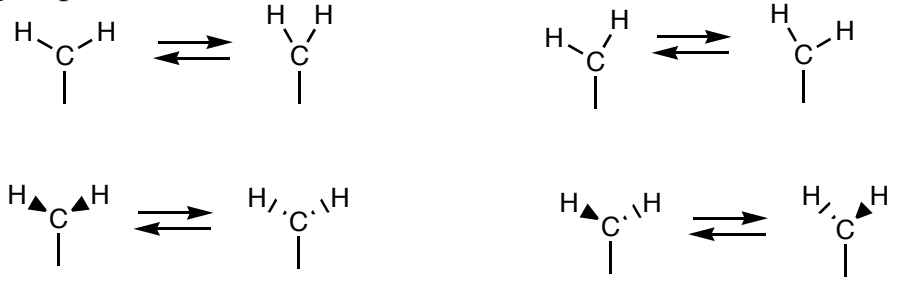
What are the two types of vibrations that molecules can undergo?

What does a stretching vibration look like in an HCl molecule?

What does a symmtrical and unsymmetrical vibration look like in a water molecule?

Which of these is the molecule actually doing?

Which of the following represent the scissor, rocking, wagging, and twisting vibrations of a CH_2 group?

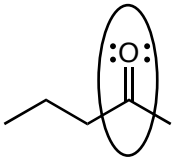


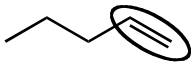
Which vibrations in a molecule will we be concerned with?

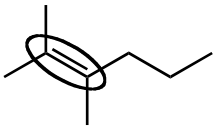
Factors which affect a band

Predict which of the following vibrations will absorb more light, and explain why.

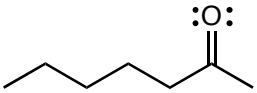
1) strength of dipole

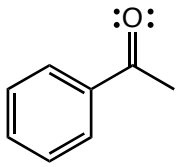






2) number of bonds



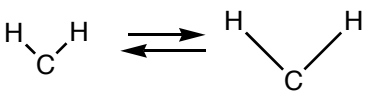


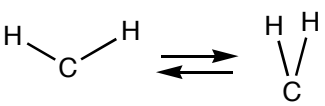
Predict which of the following bands will have the higher frequency, and explain why.

1) size of atoms C–H C–C

2) bond order C≡C C=C C–C

3) type of vibration

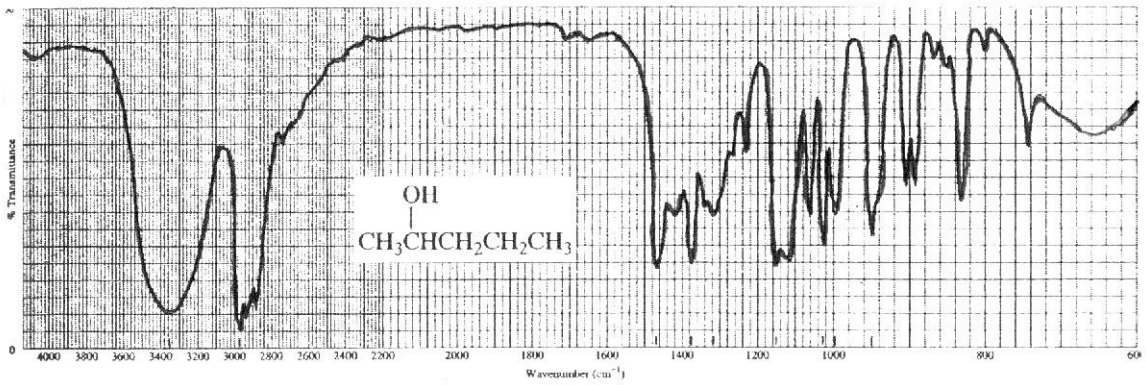


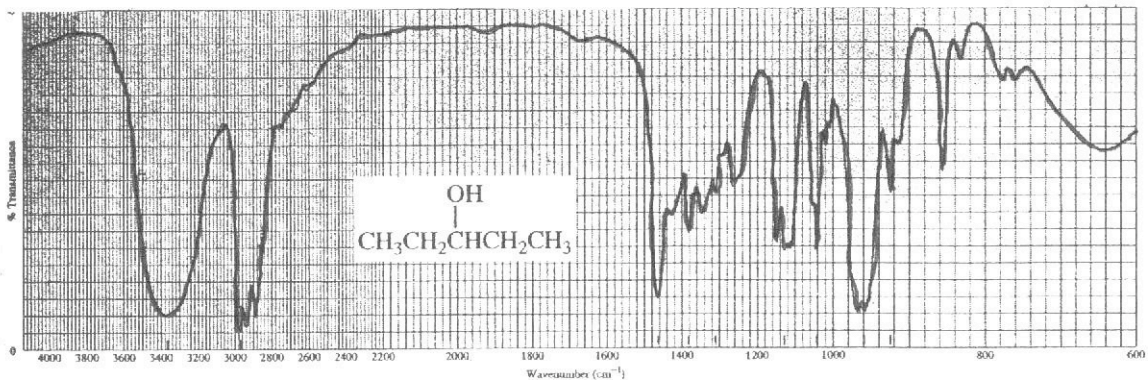


Regions of the IR Spectrum

What are the two main regions of the frequency axis?

The spectra of two different alcohols are shown below. Which bands belong tot he functional group region, and which to the fingerprint region?





If you take a spectum of an unknown compound, what can you deduce about it from the spectum?

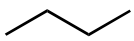
What would you need to be able to identify the compound?

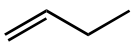
III. Identifying functional groups

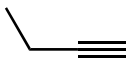
The following bonds absorb IR light at known frequencies. They are useful for deducing the functional groups of compounds.

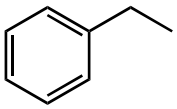
C–H	C=O	NH_2 bending
C–H on C=C	C≡N	CH_2 bending
C–H on C=O	C–O	C=C bending
C–H on C≡C	O–H	COOH dimer
C=C	O–H on C=O	aromatic overtones
C=C aromatic	N–H	
C≡C	C–X	

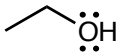
For each of the functional groups below, write down which of these bands it should have. The number of bands you should look for is given in ( ).

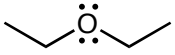
<u>alkane</u> (2) 

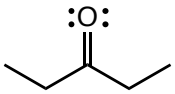
<u>alkene</u> (5) 

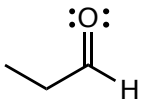
<u>alkyne</u> (4) 

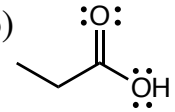
<u>aromatic ring</u> (5) 

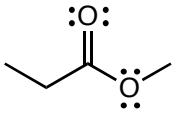
<u>alcohol</u> (4) 

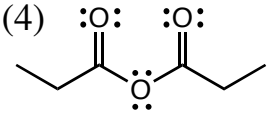
<u>ether</u> (3) 

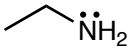
ketone (3) 

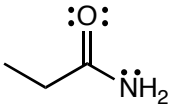
aldehyde (4) 

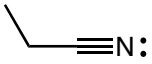
carboxylic acid (6) 

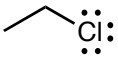
ester (4) 

anhydride (4) 

amine (4) 

amide (5) 

nitrile (3) 

alkyl halide (3) 

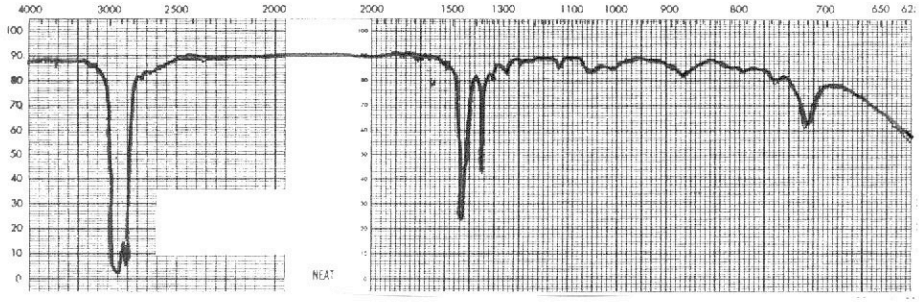
Which bands would you expect to find in the following ranges?

3400-3200 cm^{-1}	3100-2700 cm^{-1}	2250-2100 cm^{-1}	2000-1600 cm^{-1}	1300-400 cm^{-1}

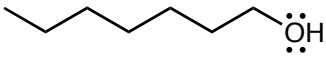
Using the charts on the previous pages, identify the important bands for each functional group.

Alkane

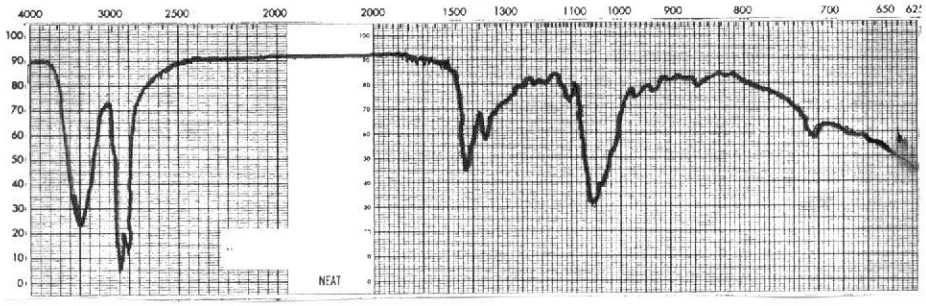
hexane



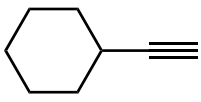
Alcohol



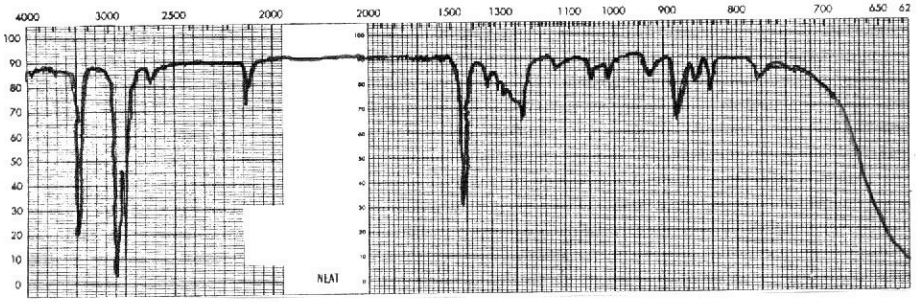
1-heptanol

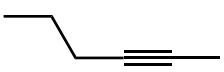


Alkyne

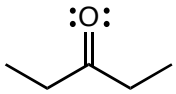


cyclohexylacetylene



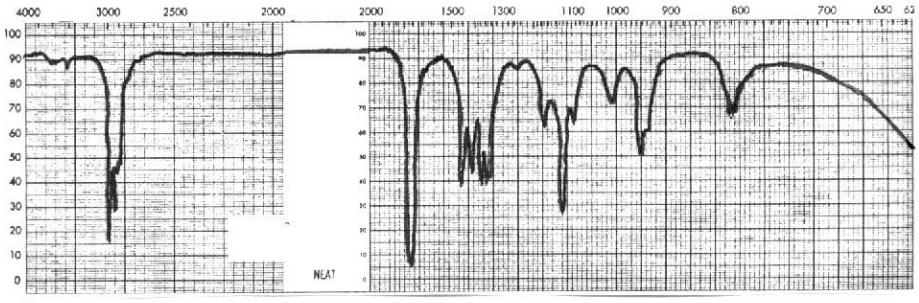


Ketone

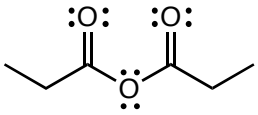


3-pentanone

expected bands:

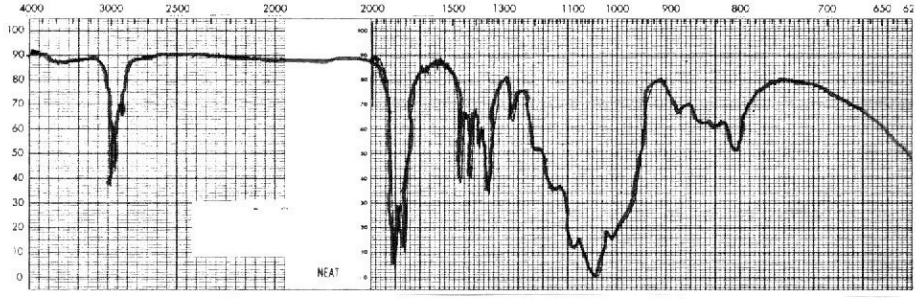


Anhydride

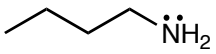


propanoic anhydride

expected bands:



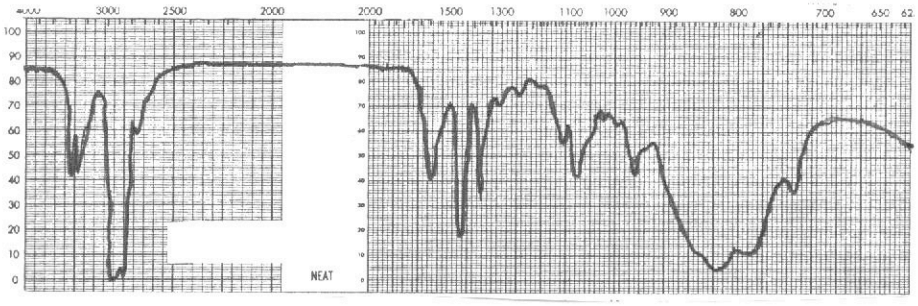
Amine

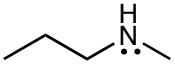


butyl amine

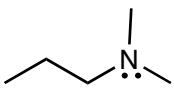
1º amine

expected bands:





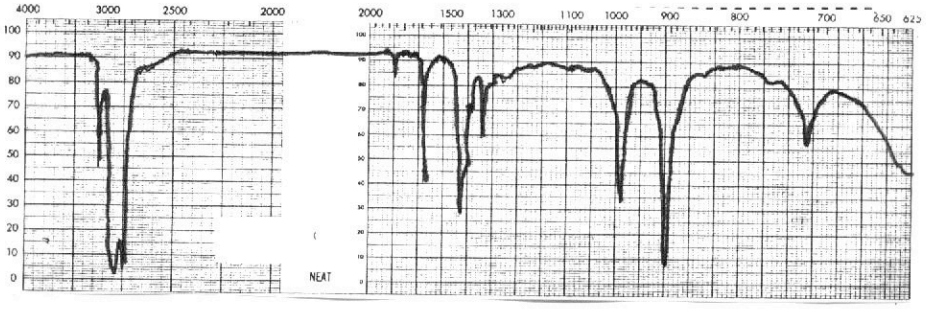
2º amine



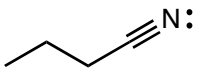
3º amine

Alkene

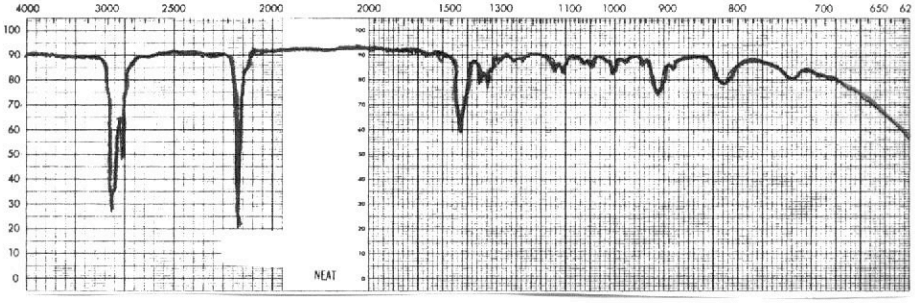
1-octene



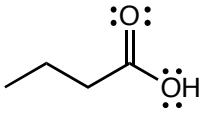
Nitrile



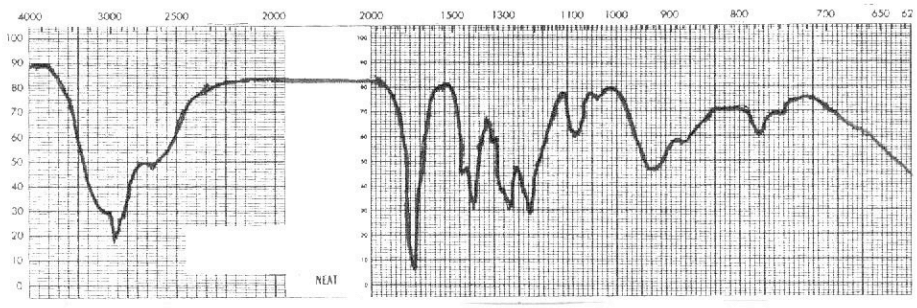
butanenitrile



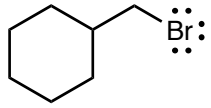
Carboxylic acid



butanoic acid

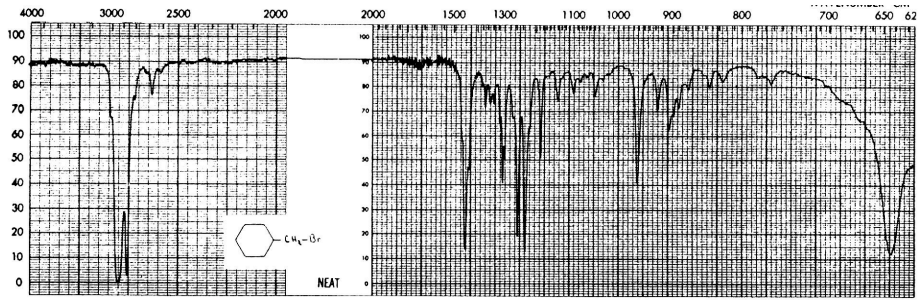


Alkyl halide

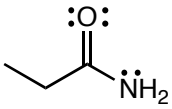


bromomethyl cyclohexane

expected bands:

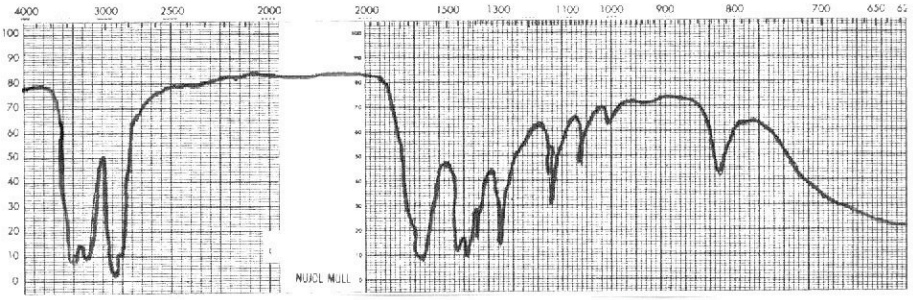


Amide

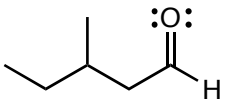


N-methylpropanamide

expected bands:

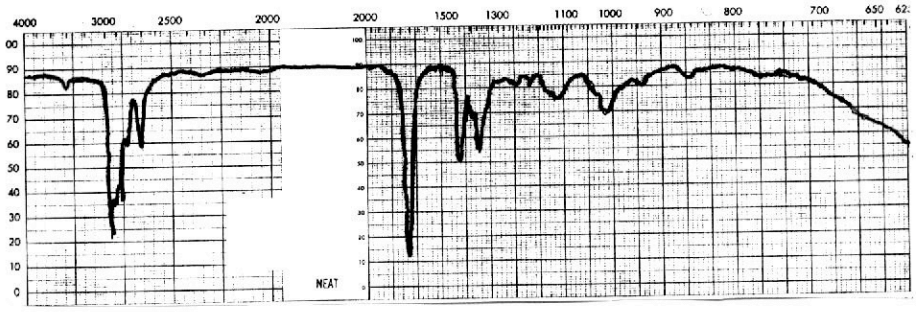


Aldehyde

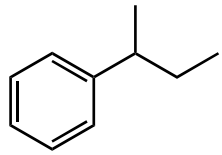


3-methylpentanal

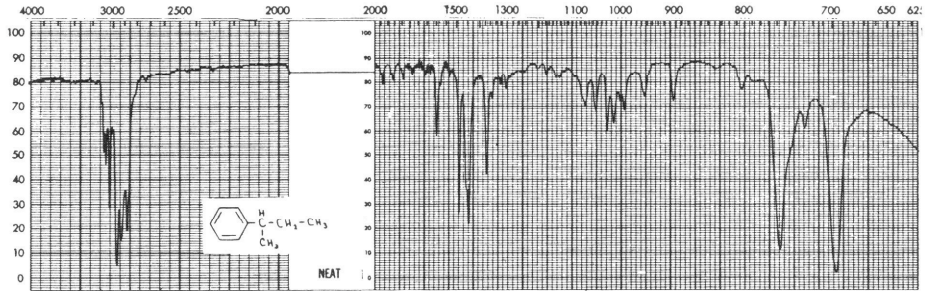
expected bands:



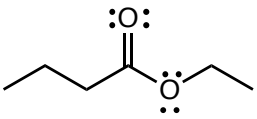
Aromatic



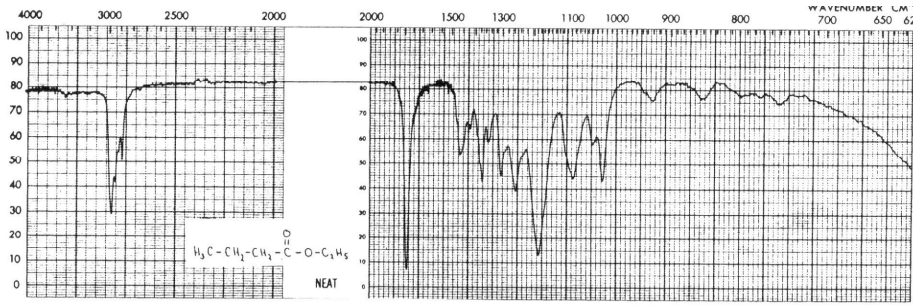
<u>sec</u>-butyl benzene



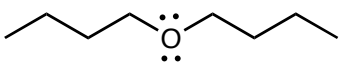
Ester



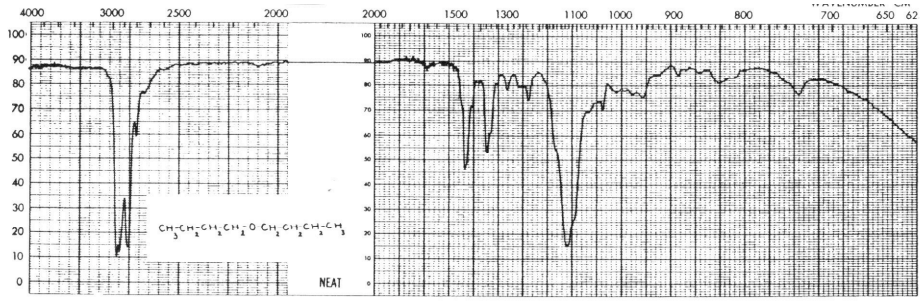
ethyl butyrate



Ether



dibutyl ether



IV. Interpreting an IR spectrum

If you think you know the identity of a compound that you have a spectrum of, what should you do?

alcohol

ester

alkene

If you don't know the identity of the compound you have a spectrum of, what should you do?

1) find C-H and CH_2 bending to use as reference points

2) look in each area for bands that stick out

3) then look for bands that confirm, or narrow it down

if you see an O-H, look for:

if you see an N-H, look for:

if you see a C $\equiv$ C or C $\equiv$ N, look for:

if you see a C=O, look for:

if there are no obvious bands, look for:

How would you tell spectra of the following compounds apart?

aldehyde vs. ketone?

alkane vs. ether?

ketone vs. ester?

amide vs. amine?

nitrile vs. alkyne?

alcohol vs. amine?

alcohol vs. carboxylic acid?

What would you look for in the IR spectum of the following reactions?