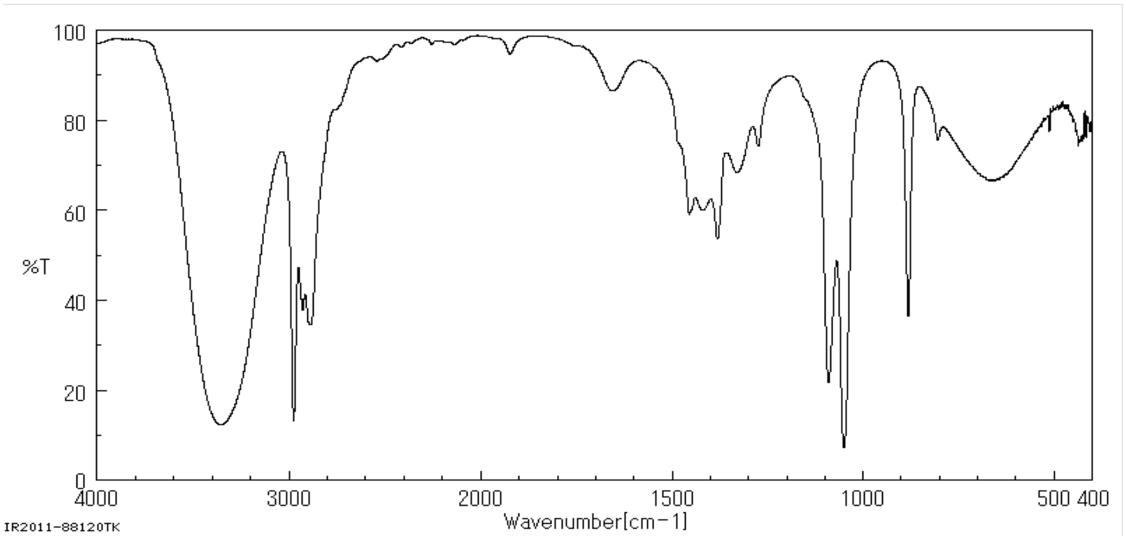
Chemistry 234

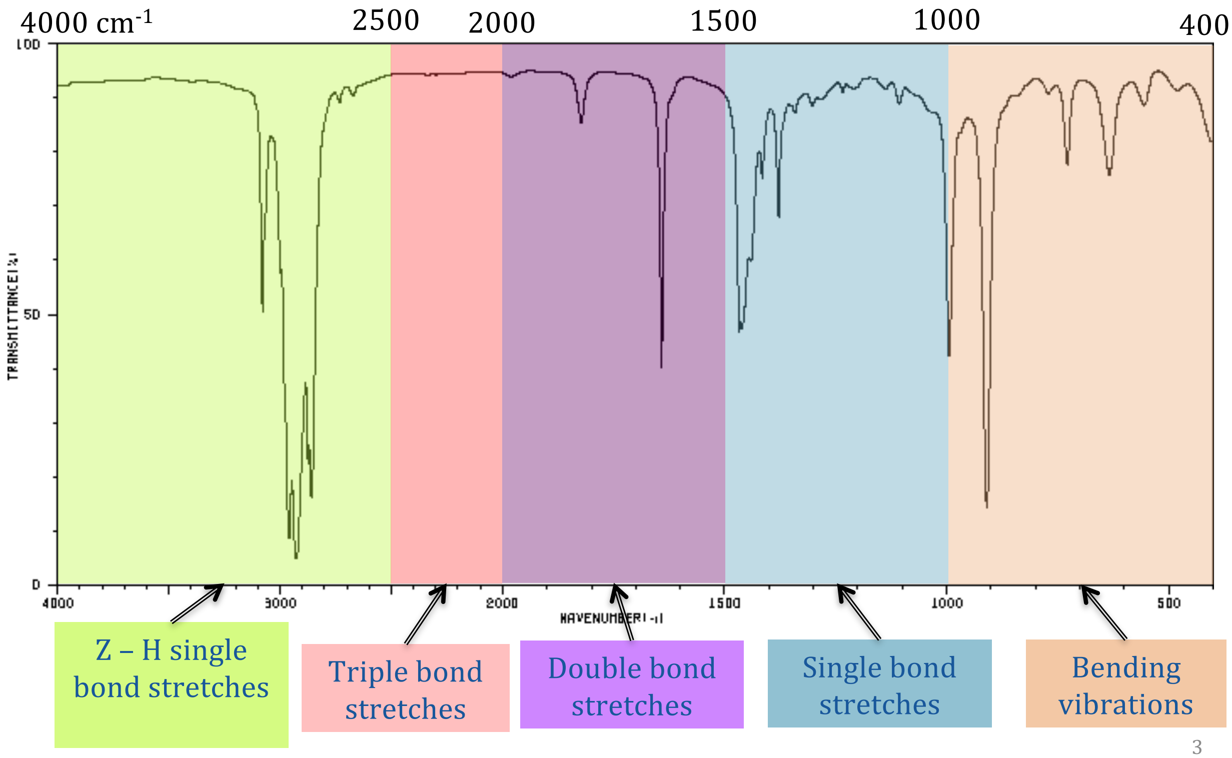
Spectroscopy Review
Spring 2019

Infrared Spectroscopy

- **Main Purpose = determination of functional groups in a molecule.**
- **Focus on the functional group region (>1500 cm^{-1}).**
- **Generally can not deduce an entire structure from IR.**



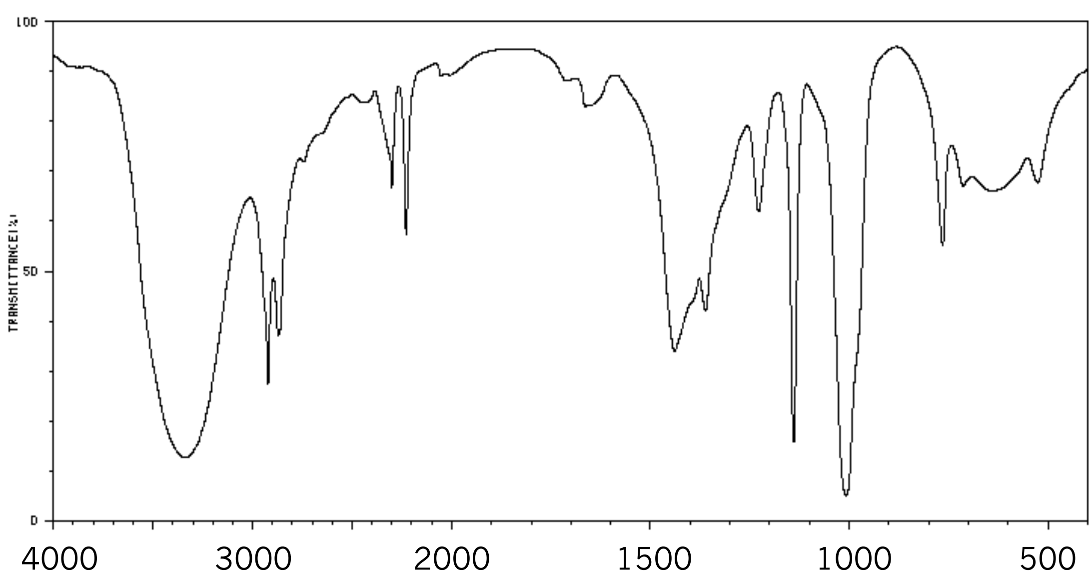
General IR Regions



Key Functional Groups to Look For

1) Alcohol O-H Stretch

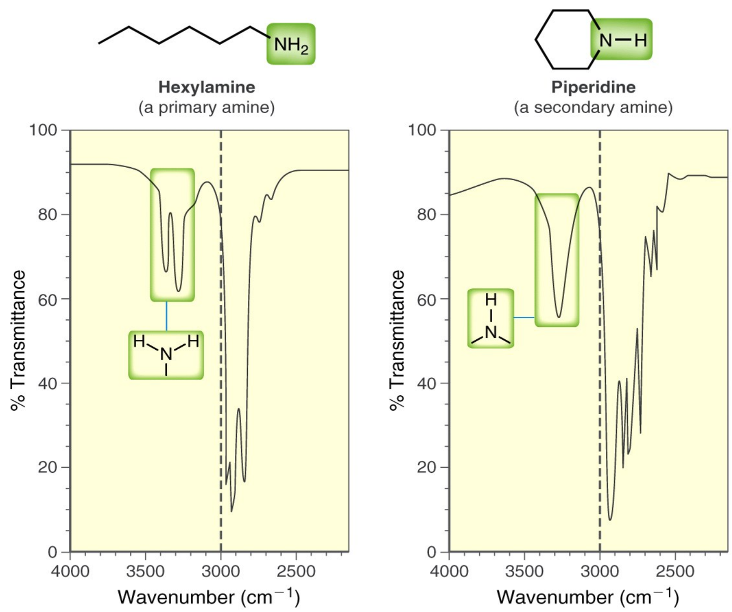
Broad Stretch, 3200-3600 cm^{-1}



Key Functional Groups to Look For

2) Amine/Amide N-H Stretch

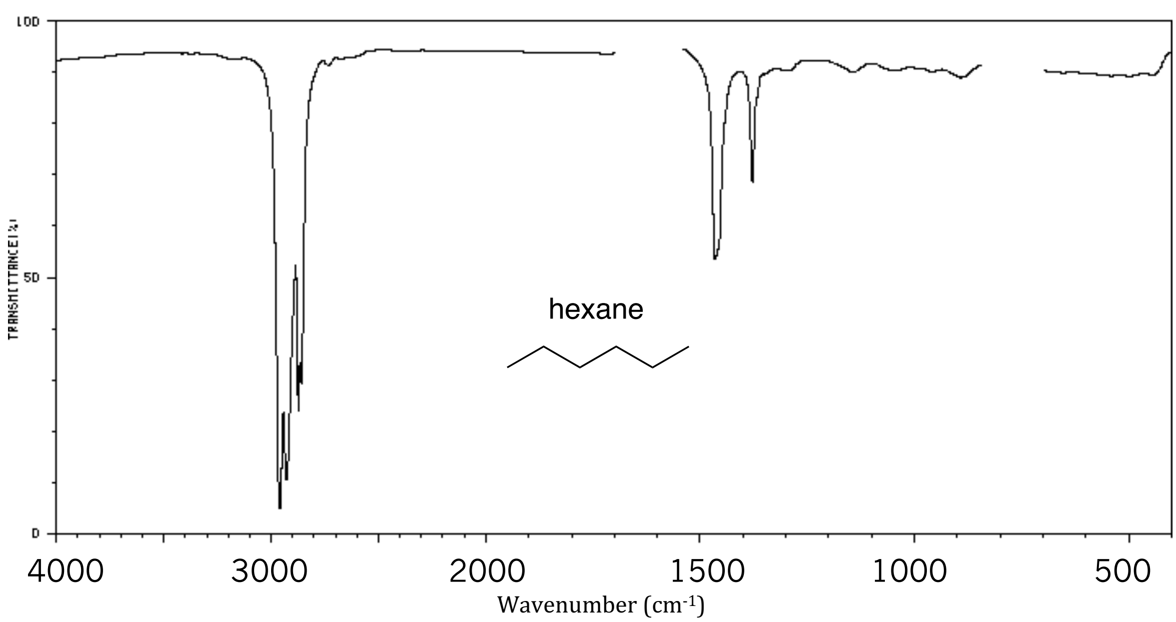
Medium Stretch, 3300-3500 cm^{-1}



Key Functional Groups to Look For

3) Alkane – Csp^3-H Stretch

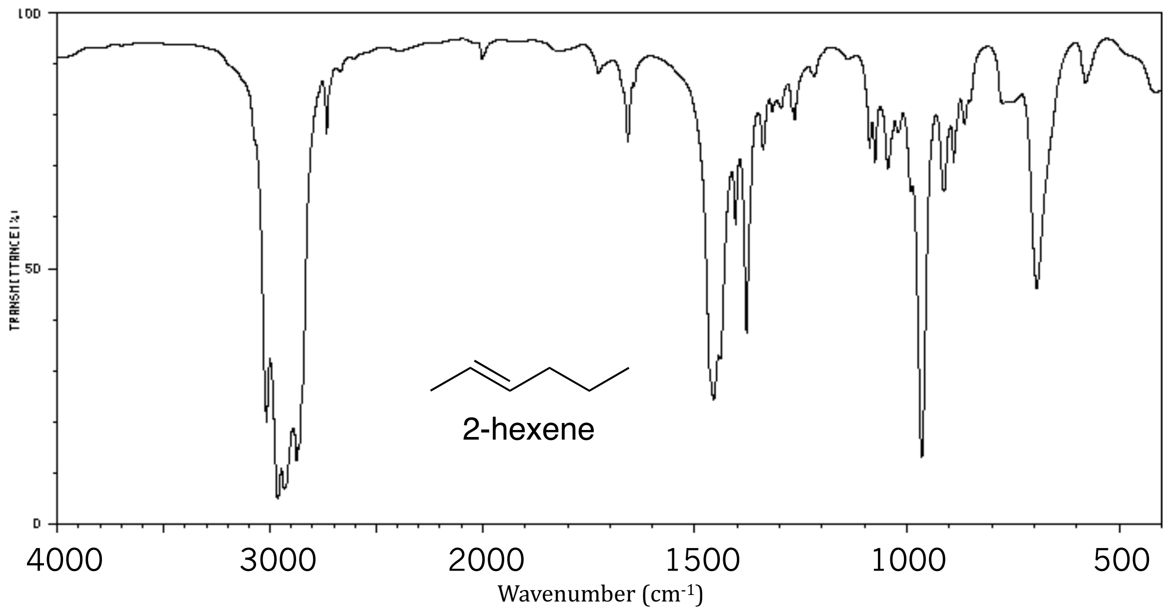
Stretches just below 3000 cm^{-1}



Key Functional Groups to Look For

4) Alkene *Csp²-H just above 3000 cm⁻¹*

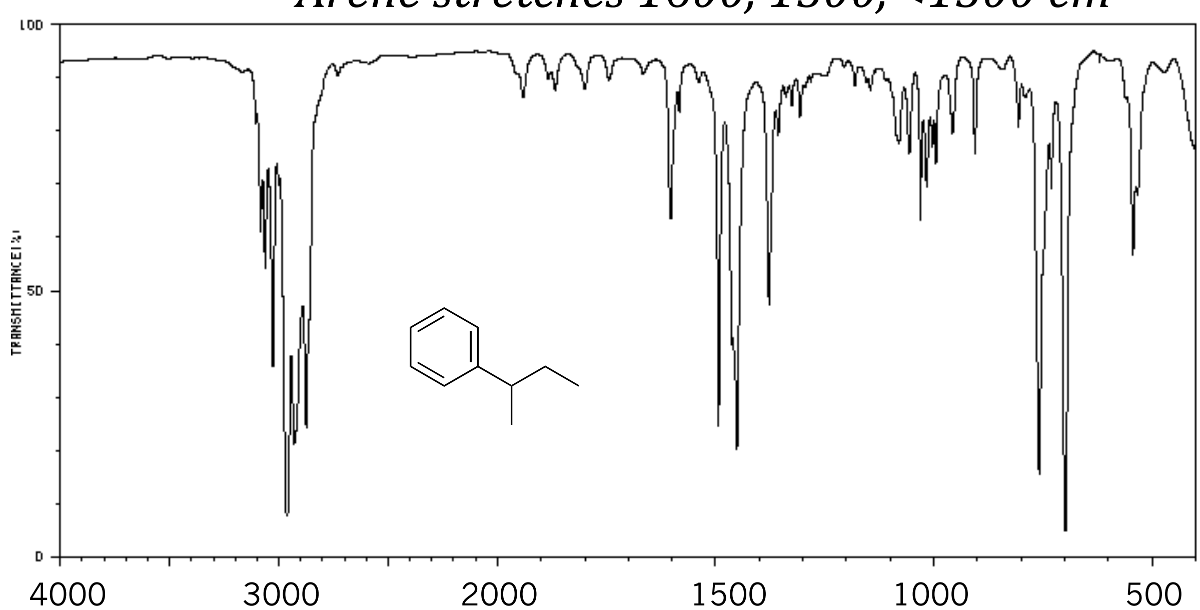
C=C stretch 1600-1700 cm⁻¹



Key Functional Groups to Look For

5) Arene *Csp²-H just above 3000 cm⁻¹*

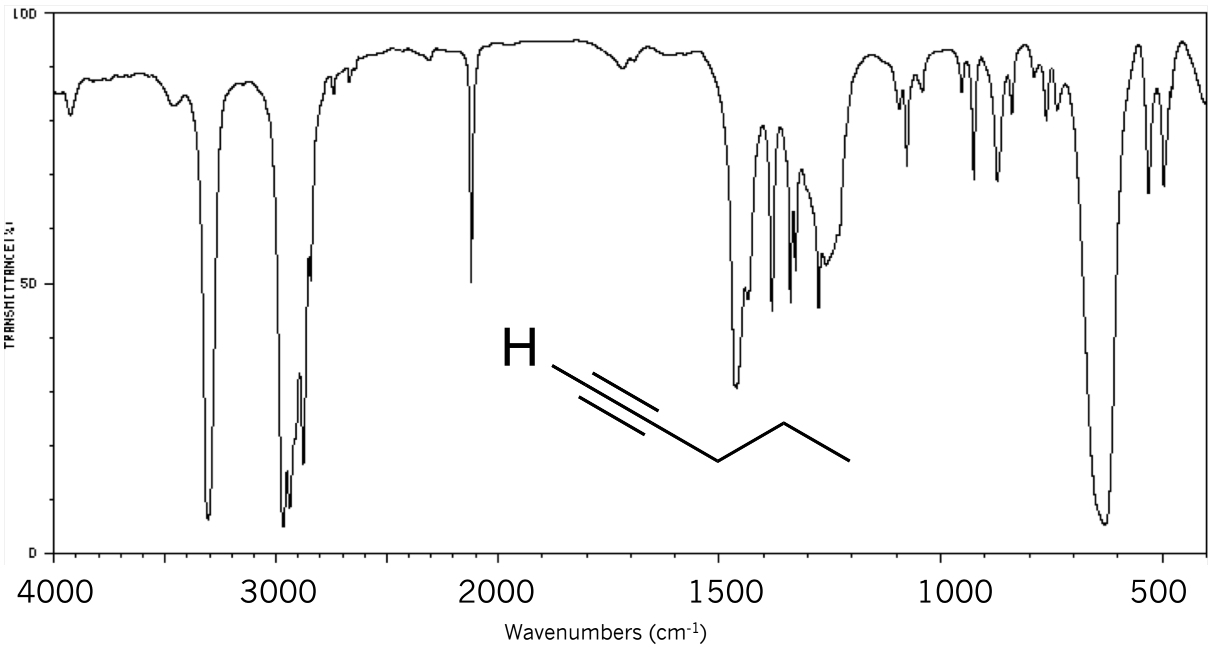
Arene stretches 1600, 1500, <1500 cm⁻¹



Key Functional Groups to Look For

6) Alkyne *Csp-H ~3300 cm^{-1} (terminal alkyne)*

C≡C stretch ~2150 cm^{-1}



Key Functional Groups to Look For

7) Carbonyl Groups

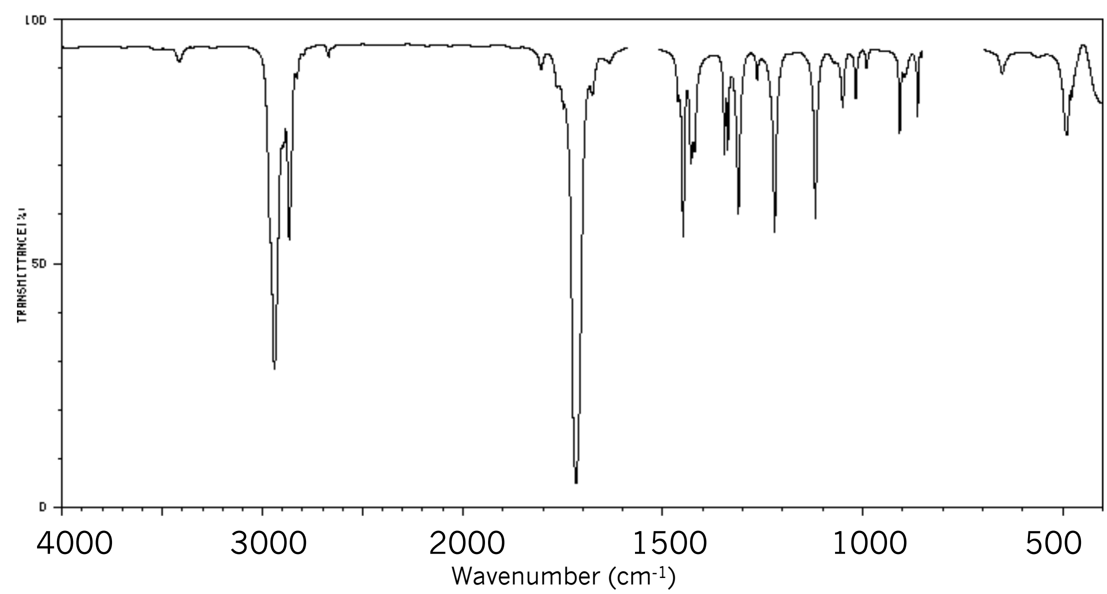
Look for the C=O functional group in the 1650 – 1750 cm^{-1} region.

Use other features to distinguish the various carbonyl groups from one another.

i.e. an amide will have a C=O stretch at 1650 cm^{-1} and NH_2 stretches around 3300 cm^{-1}

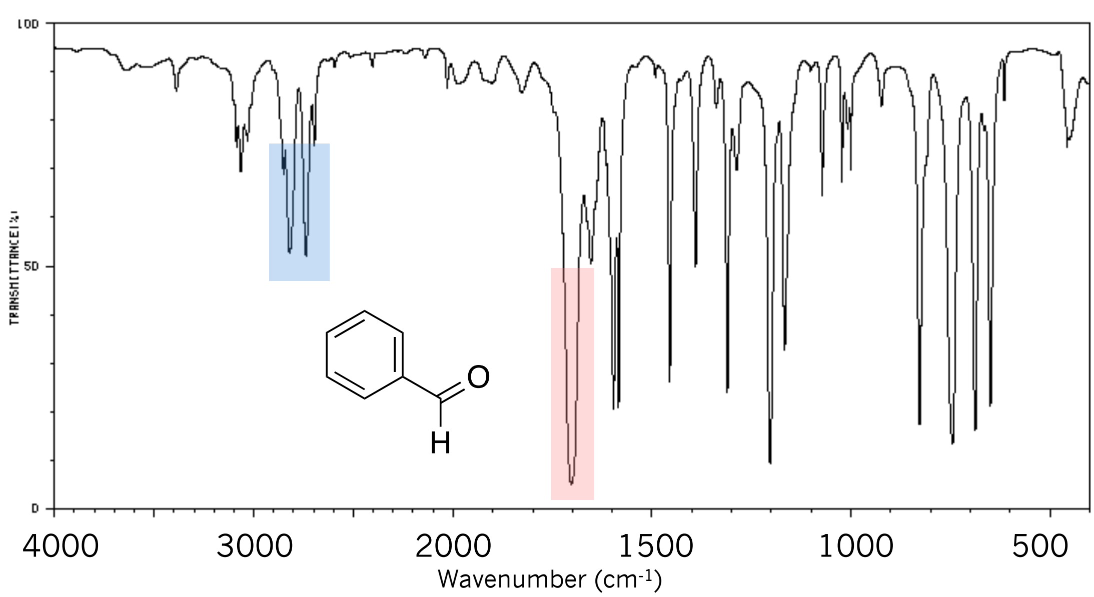
A Ketone

Strong sharp stretch ~1700 cm^{-1}



An Aldehyde

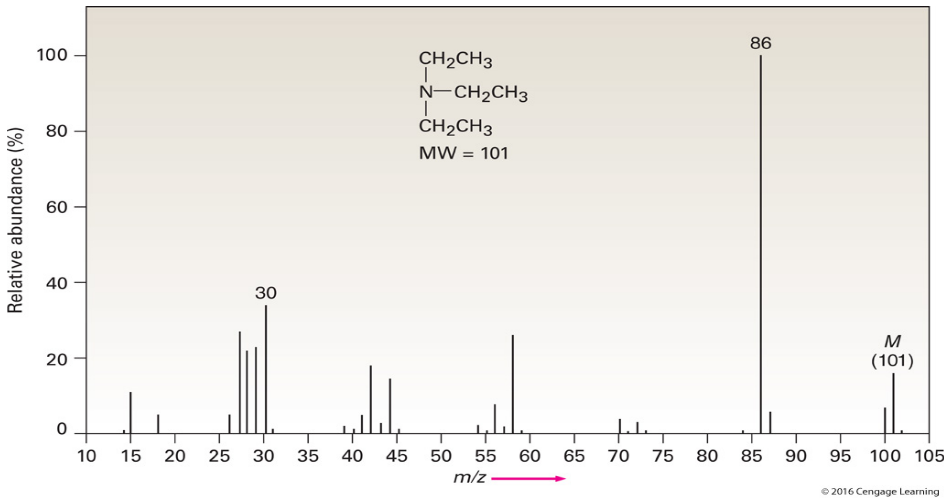
In aldehydes, look for specific aldehyde C-H stretches at ~2720 and ~2820 cm^{-1}.



Mass Spectrometry

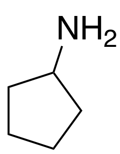
Mass Spectrometry is a technique used to elucidate the molecular formula of an organic compound.

A. Focus on the right most grouping of peaks. The tallest peak in this group is the molecular ion [M^+]. The molecular ion tells you the molecular weight.



Mass Spectrometry

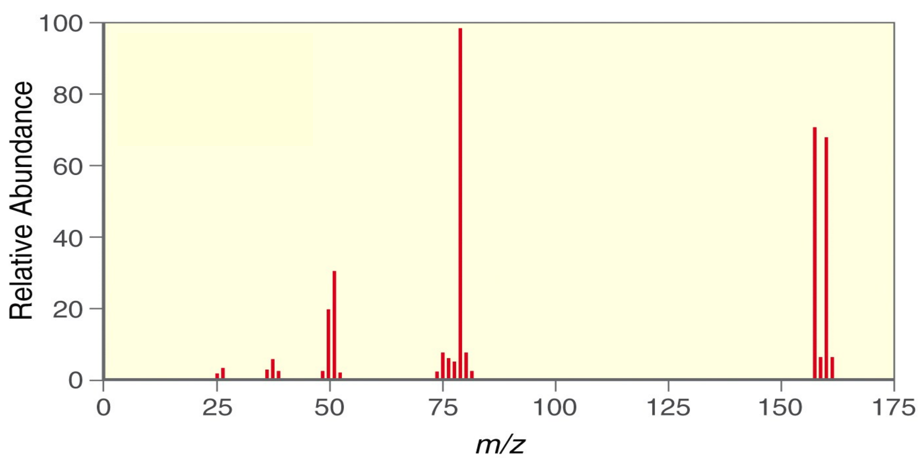
B. If the molecule has one nitrogen, the M^+ will be odd.



MW = 85 g/mol

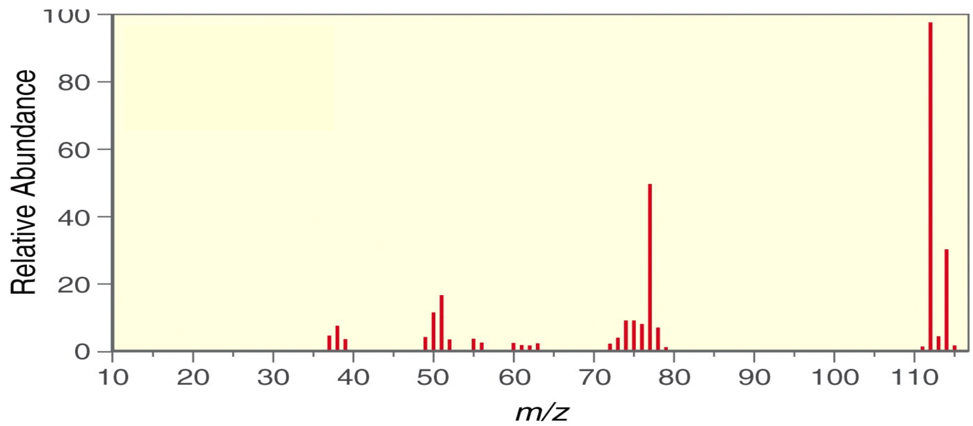
M^+ at *m/z* 85

C. An M^+ and $[M+2]^+$ in a 1:1 ratio is indicative of a Br.



Mass Spectrometry

D. An M^+ and $[M+2]^+$ in a 3:1 ratio is indicative of a Cl.



E. Rule of 13 – used to estimate carbon count

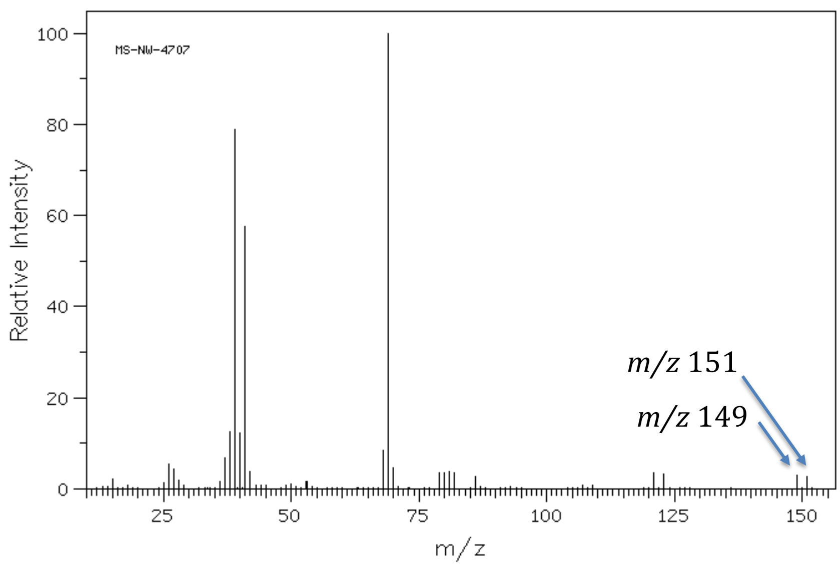
$$\#C = \frac{M^+ - \text{mass of heteroatoms}}{13}$$

< x.8 round down

Mass Spectrometry Example

Determine the molecular formula for the following:

IR Spectroscopy indicates the presence of a ketone.



Proton NMR Spectroscopy

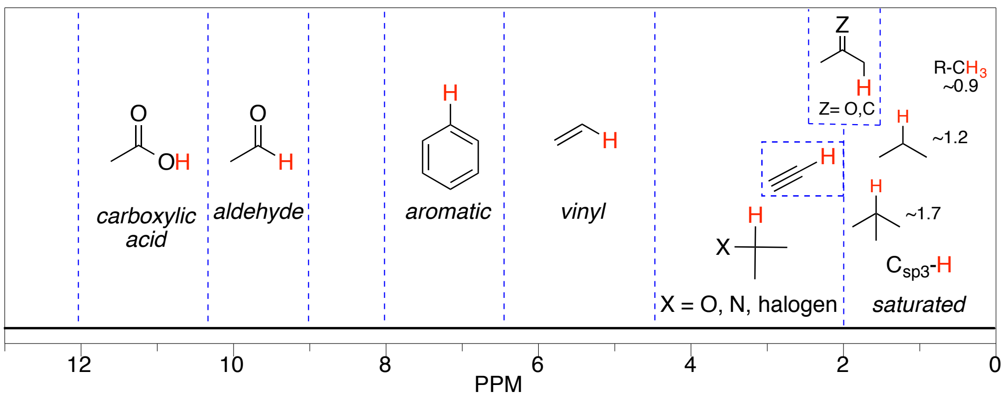
A. Determine degree of unsaturation from molecular formula.

$$DOU = \frac{2(\#C) + 2 - \#H - \#X + \#N}{2}$$

B. Write out fragments for each signal on the spectrum.

C. Determine connectivity using the chemical shift data and multiplicity.

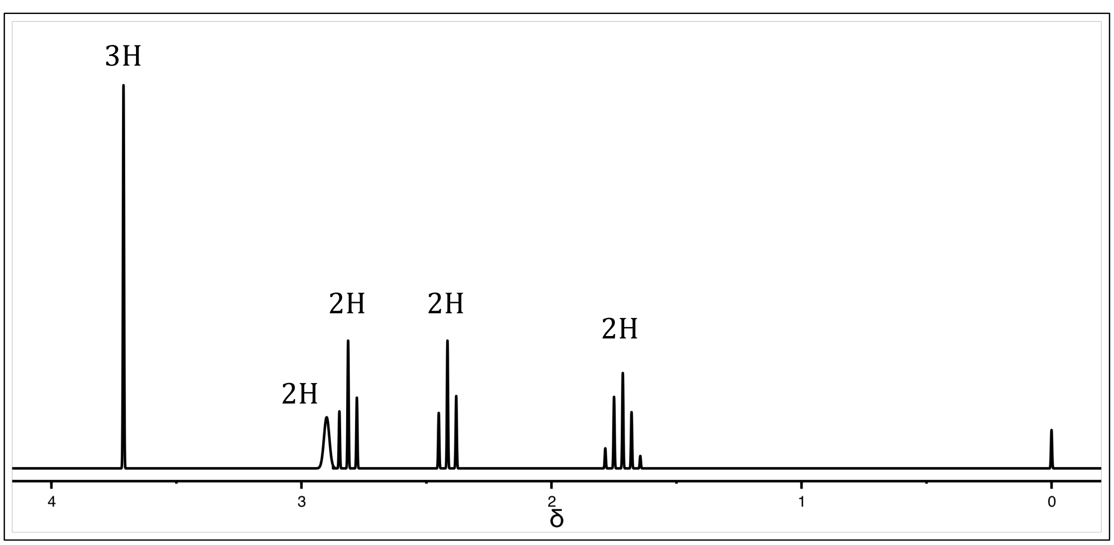
Splitting follows n+1 rule where n = #H on the neighboring carbon(s).



^{1}H NMR Example

IR shows a strong signals at 1750, 3350, 3380 cm^{-1}

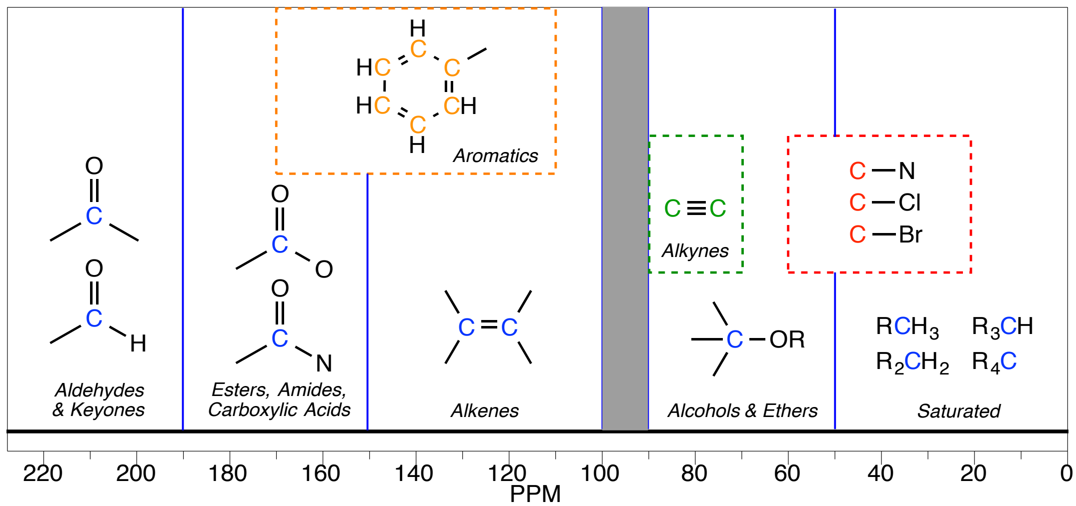
$C_5H_{11}NO_2$



^{13}C NMR

- A signal is produced for every chemically distinct carbon atom.
- Since Carbon-13 is only present in 1.1% abundance, it takes much longer to acquire a carbon NMR spectrum than a proton NMR spectrum.
- It is difficult to get accurate integration values from Carbon-13 NMR.
- Don't usually set instrument to obtain coupling information in C-13 NMR.

Basic ^{13}C Chemical Shift Regions:



^{13}C NMR Example

- Carbon 13 NMR is most often used in conjunction with proton NMR to provide additional details for the structure being elucidated.