

# How to Interpret an IR Spectrum

The IR may be broken down into 5 distinct regions.

**I. 3100-3600cm<sup>-1</sup>. Alcohols, Carboxylic Acids, Amines and Terminal Alkynes absorb here.**

The shape and exact location of the absorbance define which group is present.

Alcohols are broad, rounded and distinct around 3300cm<sup>-1</sup>.

Carboxylic Acids also broad but shift toward 3000cm<sup>-1</sup> and run into region II.

Amines are usually sharp, primary amines give double point at 3300-1

Terminal alkyne are very narrow and sharp, around 3200 cm<sup>-1</sup>

**II. 2800-3100cm<sup>-1</sup>. Carbon – hydrogen bonds absorb here.**

Alkanes absorb 2800-3000 cm<sup>-1</sup>, Alkene C-H 3100-3000cm<sup>-1</sup>

Aromatic C-H shorter and 'spikey'

**III. 2100-2400cm<sup>-1</sup>. Triple bonds absorb here.** This area is normally blank.

-C≡C- 2100-2300

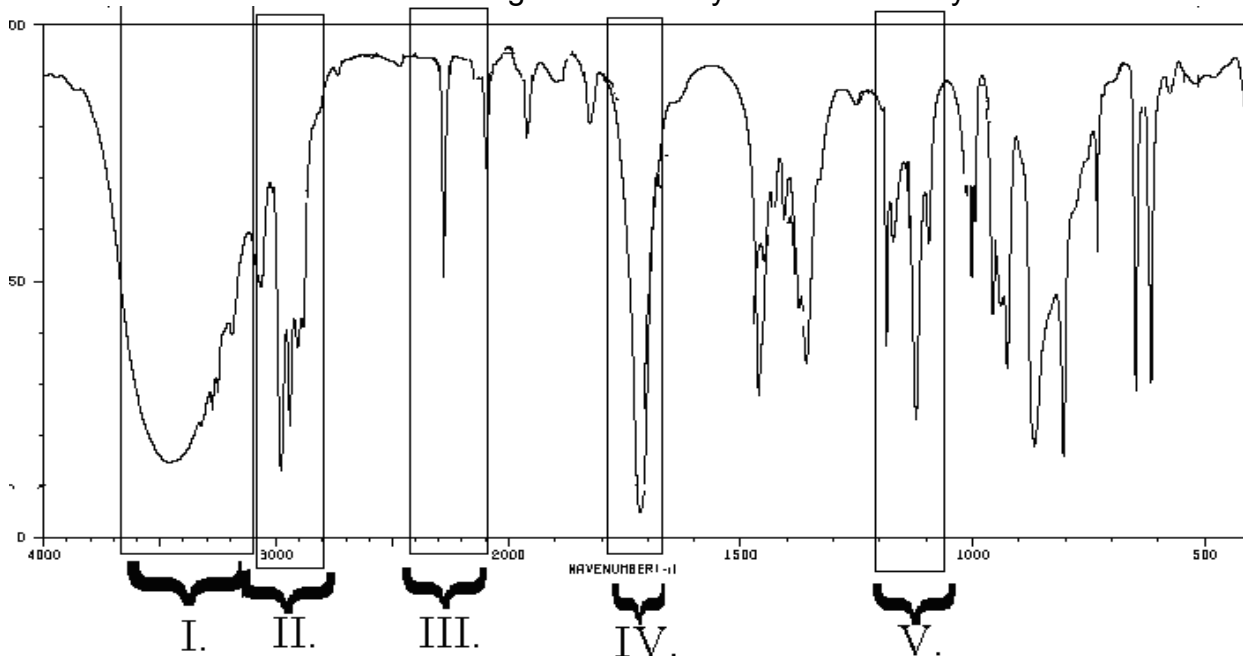
-C≡N 2200-2300

**IV. 1680-1800cm<sup>-1</sup>. Carbonyl Groups absorb here.**

-C=O very distinct strong and narrow absorbance

**V. 1050-1200cm<sup>-1</sup>. Carbon-Oxygen single bonds absorb here.**

This area is difficult to distinguish. Use only when necessary.



Region	Position (cm <sup>-1</sup> )	Functional Groups
I.	3100-3600	-OH, -NH-, ≡C-H
II.	2800-3100	-C-H
III.	2100-2400	-C≡C-, -C≡N
IV.	1680-1800	-C=O
V.	1050-1200	-C-O-

Spectra from SDBSWeb : <http://riodb01.ibase.aist.go.jp/sdbs/> (National Institute of Advanced Industrial Science and Technology, 09/20/2007)

## Region I. 3100-3600cm<sup>-1</sup>

Alcohols, Carboxylic Acids, Amines, Terminal Alkynes

**ALCOHOLS** have very distinctive **broad** absorbance around 3300 cm<sup>-1</sup>

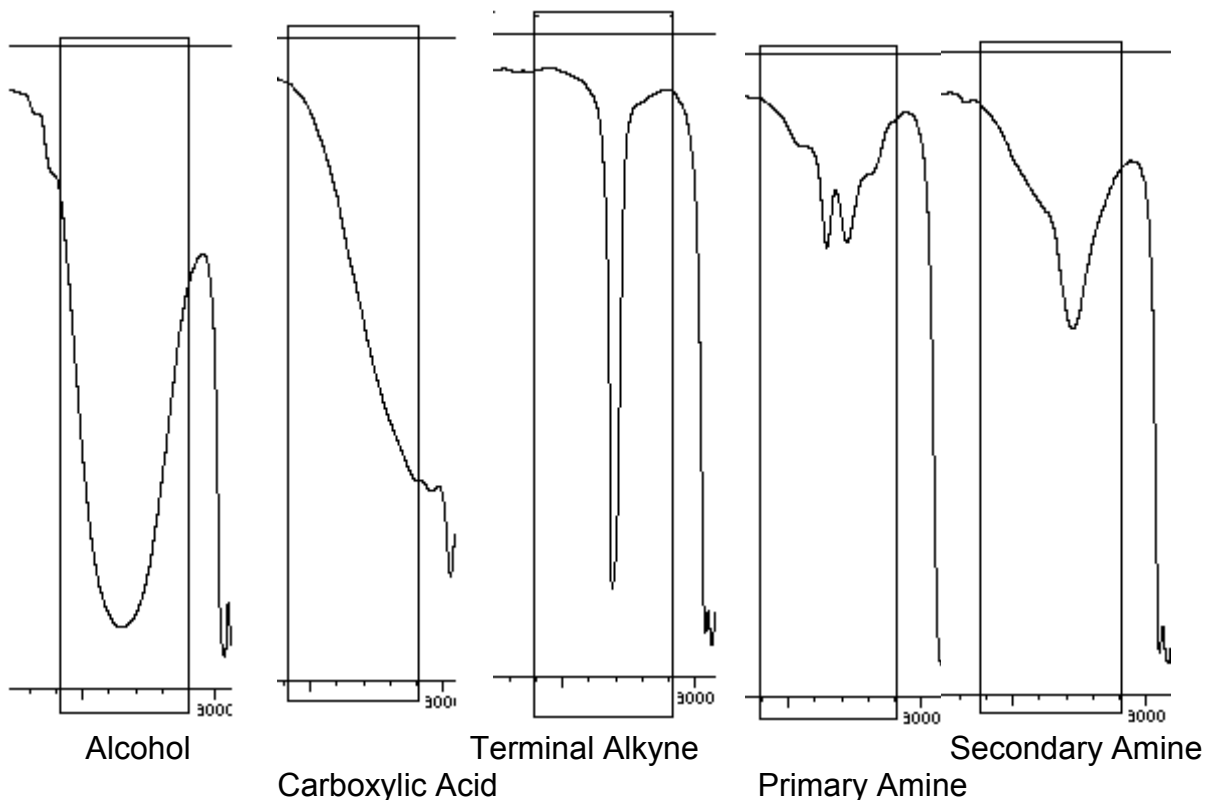
**CARBOXYLIC ACID**- The -OH of a carboxylic acid **shifts over toward 3000cm<sup>-1</sup>**.  
The -OH peak overlaps with region II

**TERMINAL ALKYNES**- The C-H bond of  $\equiv$ C-H bond has a **very sharp** needle like absorbance around 3200cm<sup>-1</sup>.

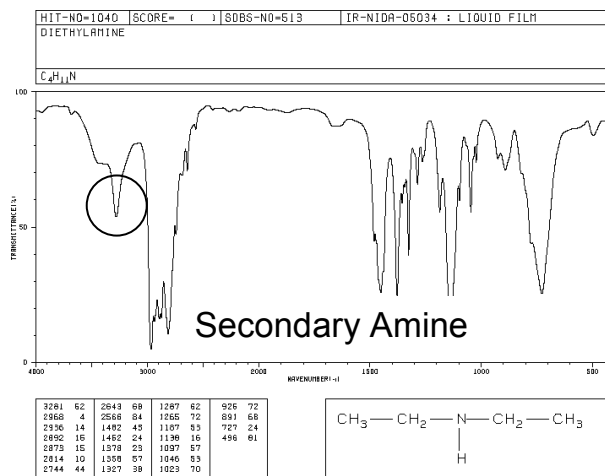
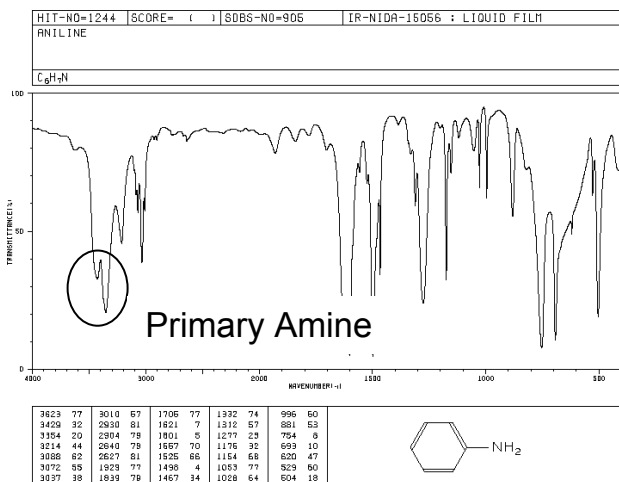
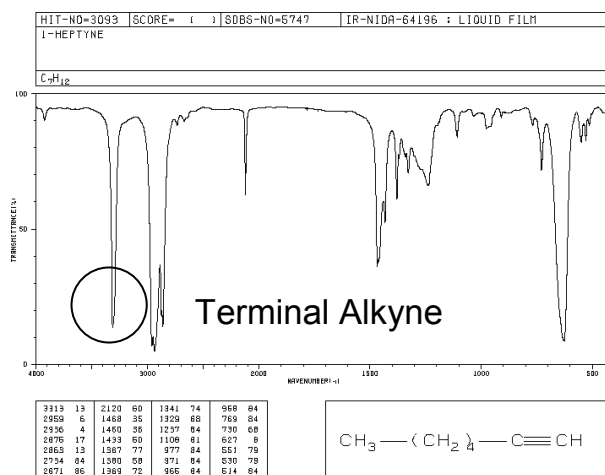
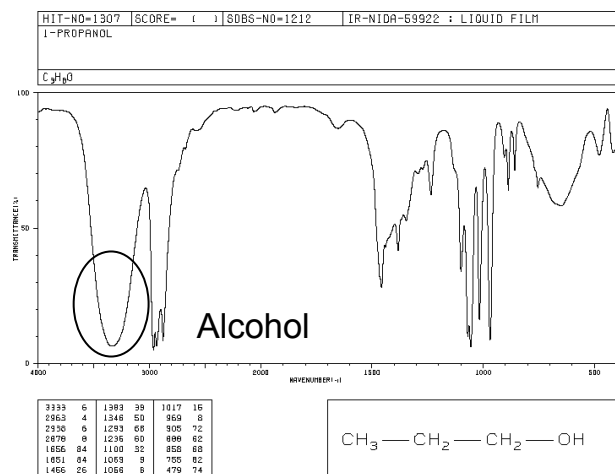
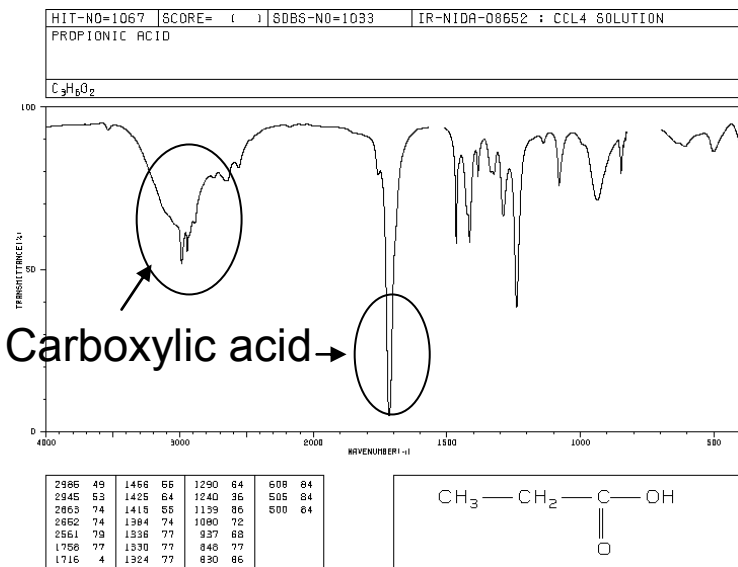
**PRIMARY AMINES**- The TWO N-H bonds show two short pointed absorbances.

**SECONDARY AMINES**- The ONE N-H bond shows one short pointed absorbance.

**TERTIARY AMINES**- There are no N-H bonds, so no absorbance in region I.



# Region I. Differences between carboxylic acids, Alcohols, Terminal Alkynes and Amines

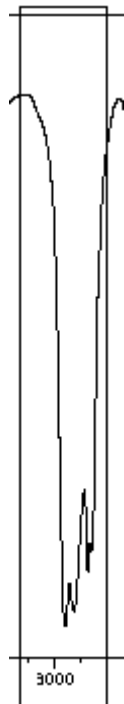


Spectra from SDBSWeb : <http://riodb01.ibase.aist.go.jp/sdbs/> (National Institute of Advanced Industrial Science and Technology, 09/20/2007)

## Region II. 2800-3100 $\text{cm}^{-1}$ . C-H bonds.

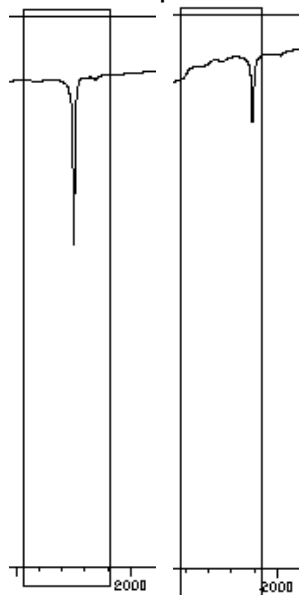
ALKANES have little discernable difference in IR.

Virtually every organic molecule will have an absorbance in this region. It is not very valuable to help distinguish structure.



## Region III. 2100-2400 $\text{cm}^{-1}$ . Triple bonds. $\text{-C}\equiv\text{N}$ or $\text{C}\equiv\text{C}$ .

ALKYNES and NITRILES have an absorbance in a usually barren area of 2100-2400 $\text{cm}^{-1}$ . The nitrile peak is usually stronger than alkyne.



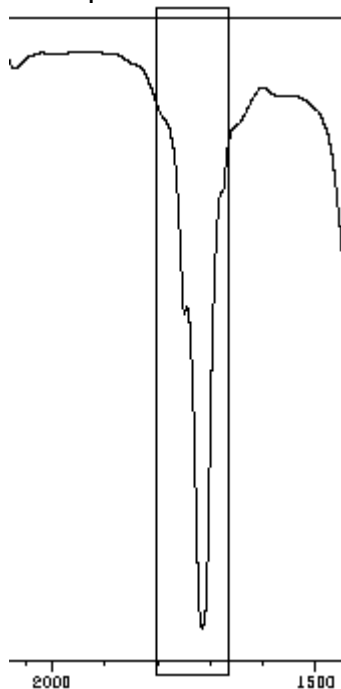
Nitrile

alkyne

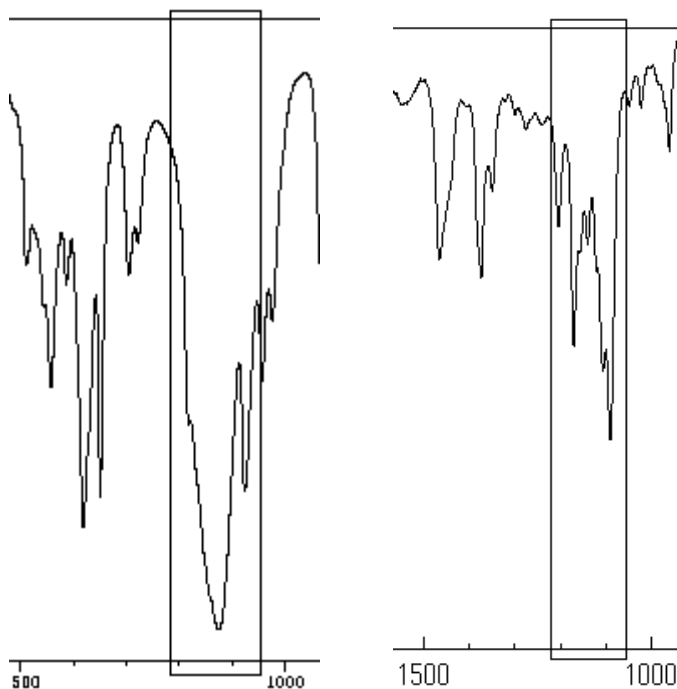
Spectra from SDBSWeb : <http://riodb01.ibase.aist.go.jp/sdbs/> (National Institute of Advanced Industrial Science and Technology, 09/20/2007)

## Region IV. 1680-1800cm<sup>-1</sup> C=O

CARBONYLS have very distinctive and strong absorbance between 1680-1800 cm<sup>-1</sup>  
2-Propanone.



**Region V. 1050-1200cm<sup>-1</sup>**. C-O stretch. Often hard to distinguish from other absorbances.



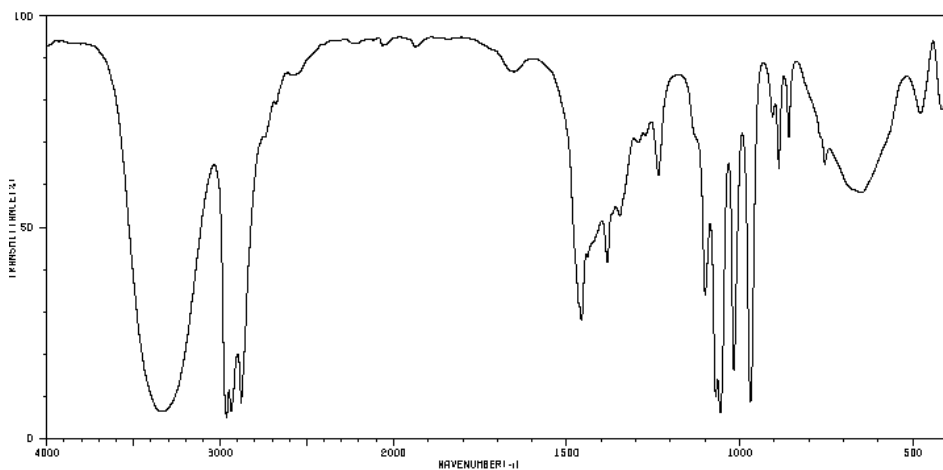
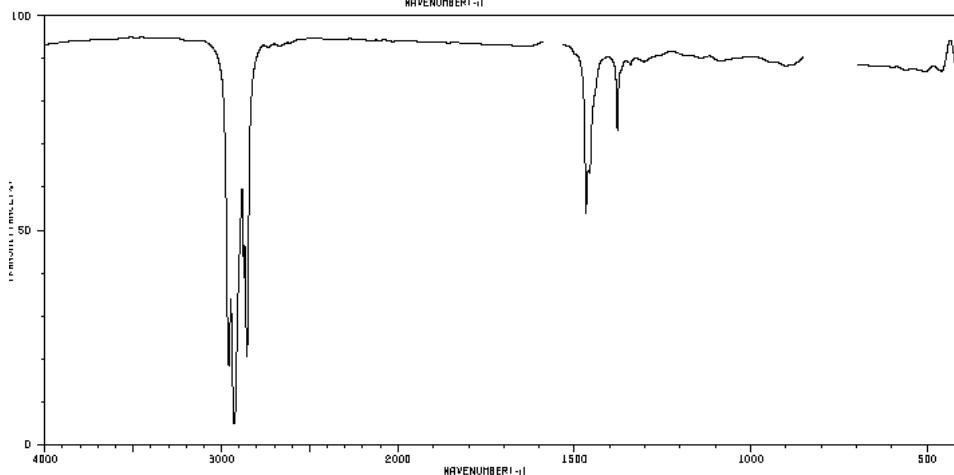
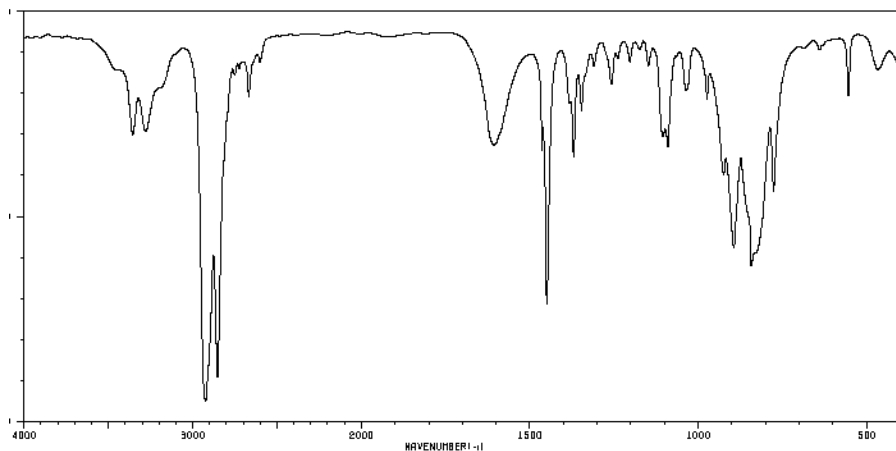
Spectra from SDBSWeb : <http://riodb01.ibase.aist.go.jp/sdbs/> (National Institute of Advanced Industrial Science and Technology, 09/20/2007)

### Matching level

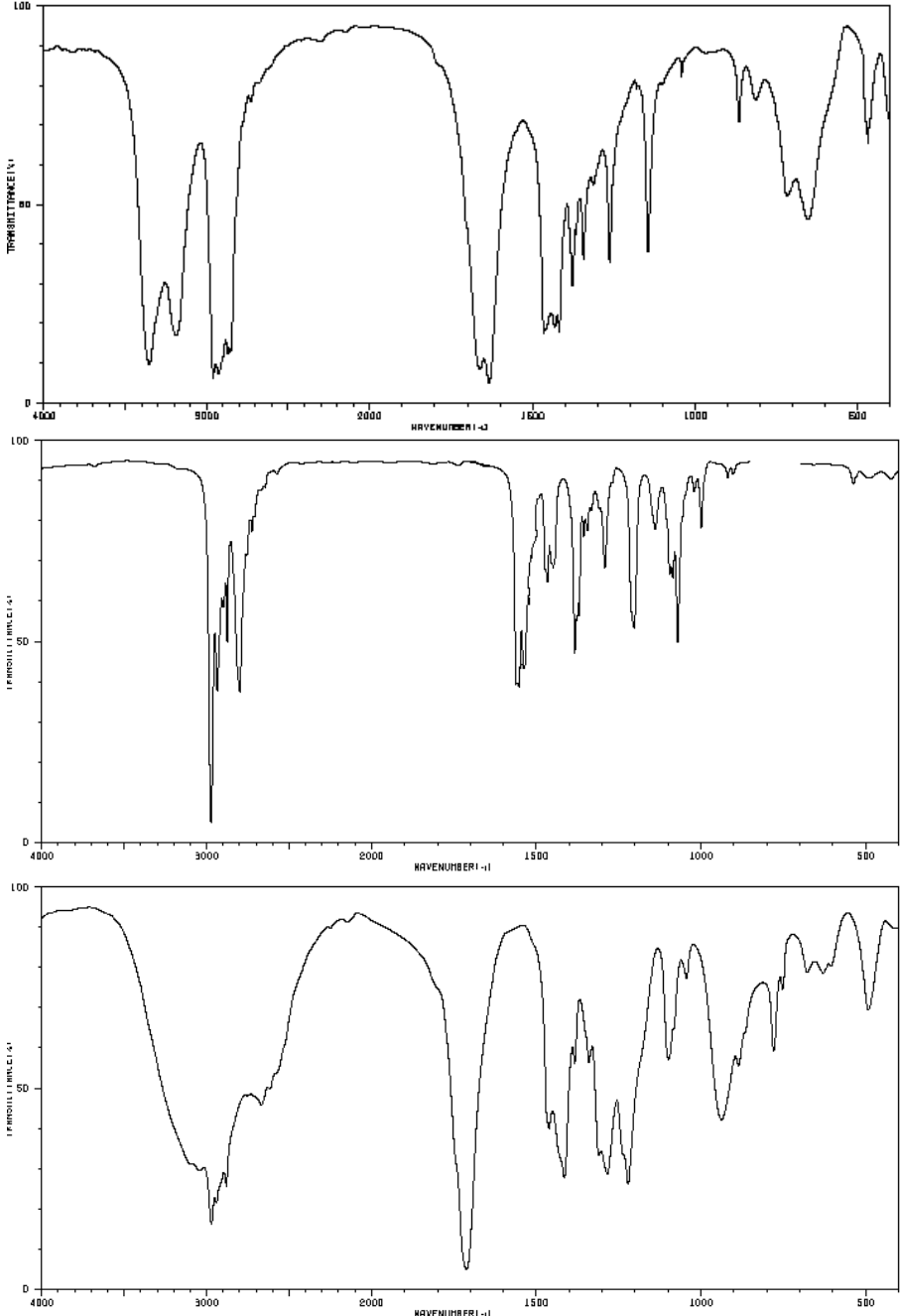
Spectra- assign a single letter to each spectra.

Functional Group (may use more than once. )

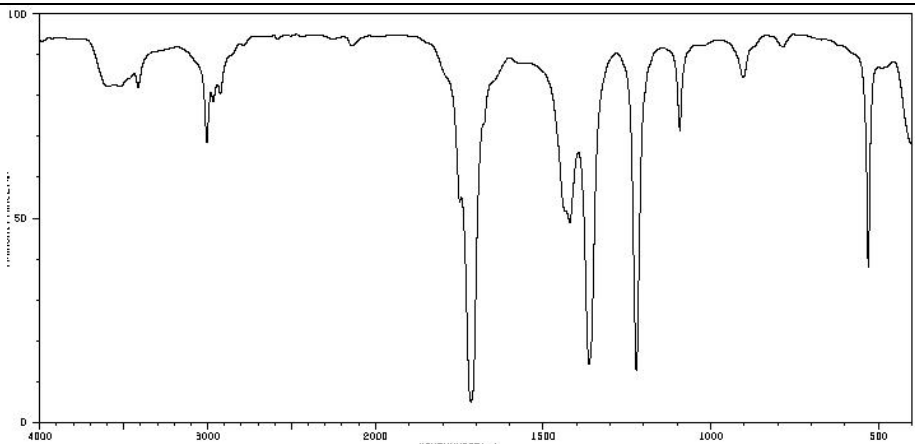
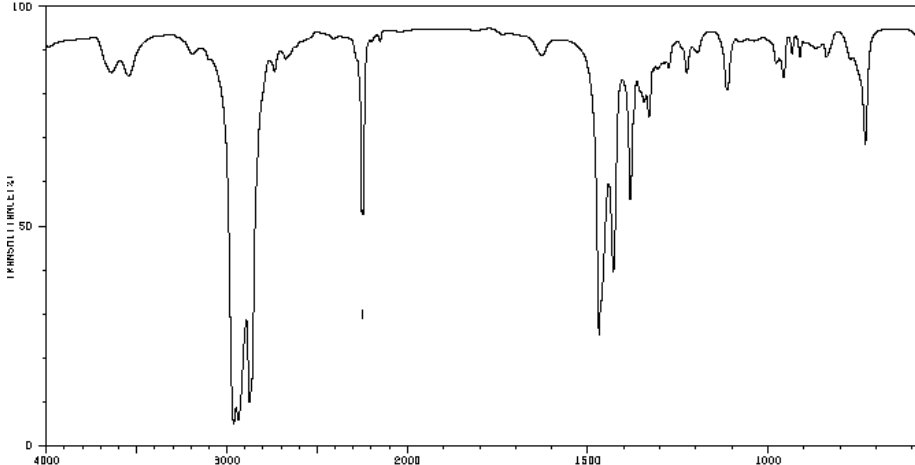
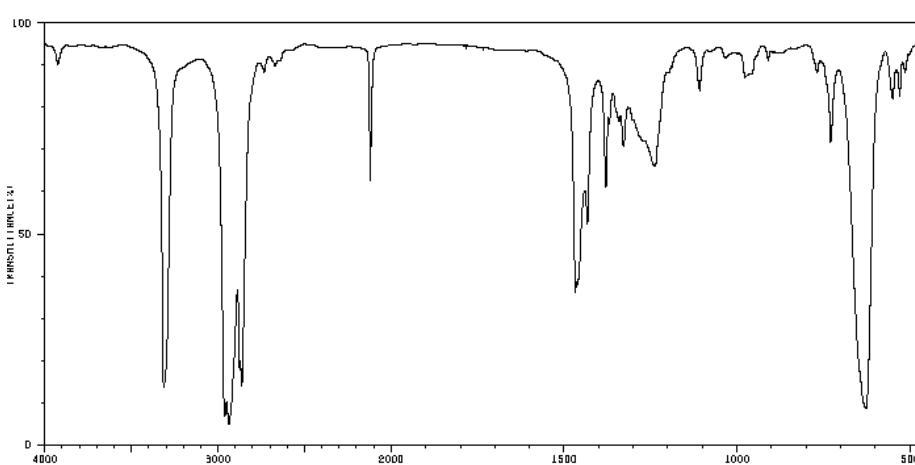
- A. Alkane
- B. Alcohol
- C. Alkyne (not terminal) or nitrile
- D. Terminal Alkyne
- E. Carboxylic Acid
- F. Primary Amine
- G. Secondary Amine
- H. Ether
- I. Ester
- J. Amide
- K. Ketone



Spectra from SDBSWeb : <http://riodb01.ibase.aist.go.jp/sdbs/> (National Institute of Advanced Industrial Science and Technology, 09/20/2007)

Spectra- assign a single letter to each spectra.	Functional Group (may use more than once.)
 <p>The image contains three IR spectra plots. Each plot shows Transmittance (%) on the y-axis (0 to 100) and Wavenumber (cm⁻¹) on the x-axis (4000 to 500).  - The top spectrum shows a broad absorption band between 3000 and 3600 cm⁻¹, a sharp peak at approximately 1700 cm⁻¹, and several peaks in the fingerprint region (1500-500 cm⁻¹).  - The middle spectrum shows a very sharp, intense peak at approximately 3000 cm⁻¹, a sharp peak at approximately 1700 cm⁻¹, and several peaks in the fingerprint region.  - The bottom spectrum shows a broad absorption band between 3000 and 3600 cm⁻¹, a sharp peak at approximately 1700 cm⁻¹, and several peaks in the fingerprint region.</p>	<ul style="list-style-type: none"> <li>A. Alkane</li> <li>B. Alcohol</li> <li>C. Alkyne (not terminal) or nitrile</li> <li>D. Terminal Alkyne</li> <li>E. Carboxylic Acid</li> <li>F. Primary Amine</li> <li>G. Secondary Amine</li> <li>H. Ether</li> <li>I. Ester</li> <li>J. Amide</li> <li>K. Ketone</li> </ul>

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