

Citrus College

Infrared Spectroscopy (IR)

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Common Functional Groups

Alkane; RCH_3

Alkene; $\text{RCH}=\text{CH}_2$

Alkyne; $\text{RC}\equiv\text{CH}$

Nitrile; $\text{RC}\equiv\text{N}$

Ether; R-O-R

Alcohol; ROH

Carboxylic Acid; RCOH



Acyl Halide; RCX (X = F, Cl, Br, I)



Acid Anhydride; RC-O-CR



Ester; RC-O-R



Amide; RC-NH_2 (1°)



RC-NH-R (2°)



RC-N-R (3°)



Aldehyde; RCH



Ketone; RCR



Amine; RNH_2 (1°)

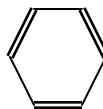
RNHR (2°)

RNR (3°)



Alkyl Halide; RCH_2X

Aromatic;



Spectroscopy & the Electromagnetic Spectrum:

Spectroscopy is the study of the interaction of matter & electromagnetic radiation:

10^{19}	10^{17}	10^{15}	10^{13}	10^{10}	10^3	ν (Hz)
γ Ray	X Ray	UV	Visible	IR	Microwave	Radio Wave
10^{-6}	10^{-4}	10^{-1}	0.4	0.8	10^2	10^6 10^{10}
						λ (μm)

ν = frequency (cycles/s)

λ = wavelength

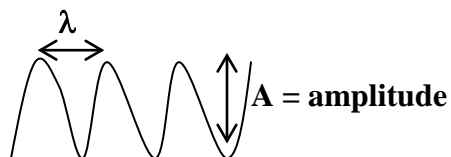
$\nu = c/\lambda$

c = speed of light = 3.00×10^{10} m/s

$E = h\nu$

E = Energy (KJ/mol)

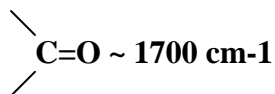
h = Planck's constant



The electromagnetic radiation can be described either by its frequency (ν) or its wavelength (λ). Wavenumber ($\tilde{\nu}$) is the third unit used to describe electromagnetic radiation. $\tilde{\nu} = 1/\lambda$ (cm^{-1})

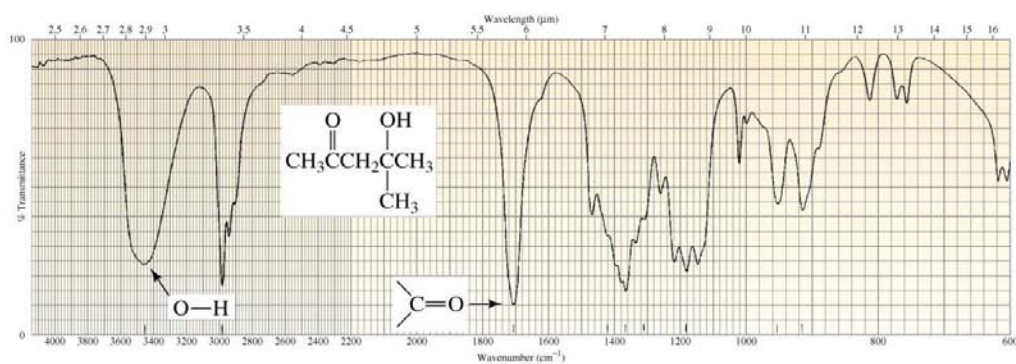
The bonds in an organic molecule are constantly vibrating. The bonds vibrate with both stretching & bending motions. There are symmetric & asymmetric stretches & bends. Each stretching & bending vibrations of a bond occurs with certain frequency. When a compound is bombarded with IR frequency, the bonds stretch & bend a bit more. The “A = Amplitude” increases. By experimentally determining the λ of the absorbed light, we can determine the kind of bond.

Stretching vibration:



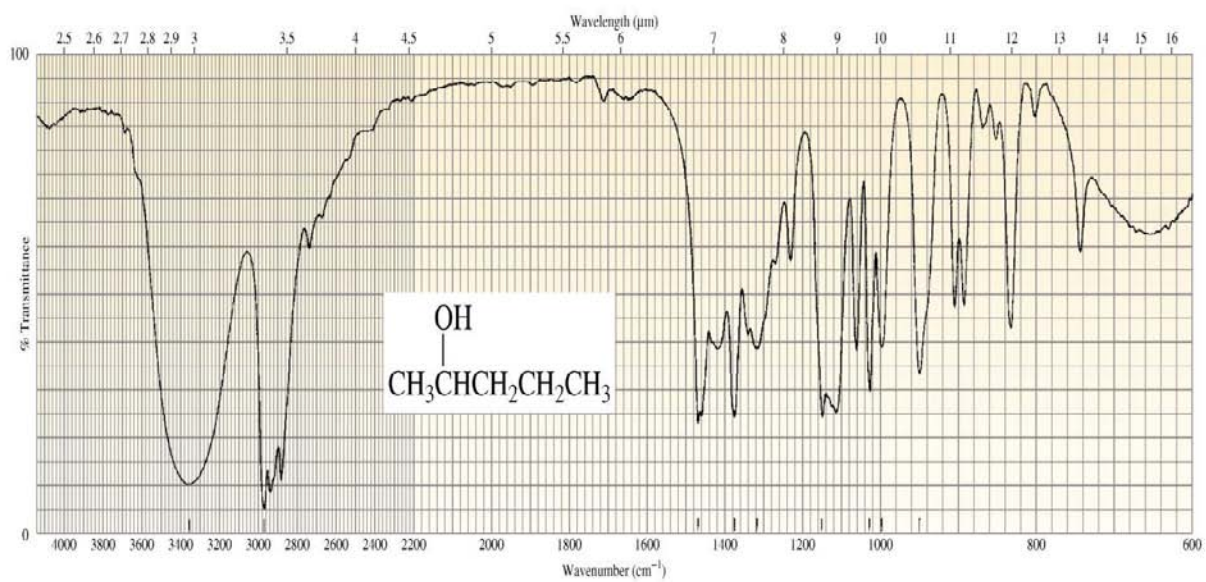
$-\text{O}-\text{H} \sim 3450 \text{ cm}^{-1}$

An IR Spectrum is obtained by passing a beam of IR radiation ($\tilde{\nu} = 4000 \text{ cm}^{-1} - 400 \text{ cm}^{-1}$) through a sample. A detector generates a plot of %Transmission vs. the $\tilde{\nu}$ (or λ).

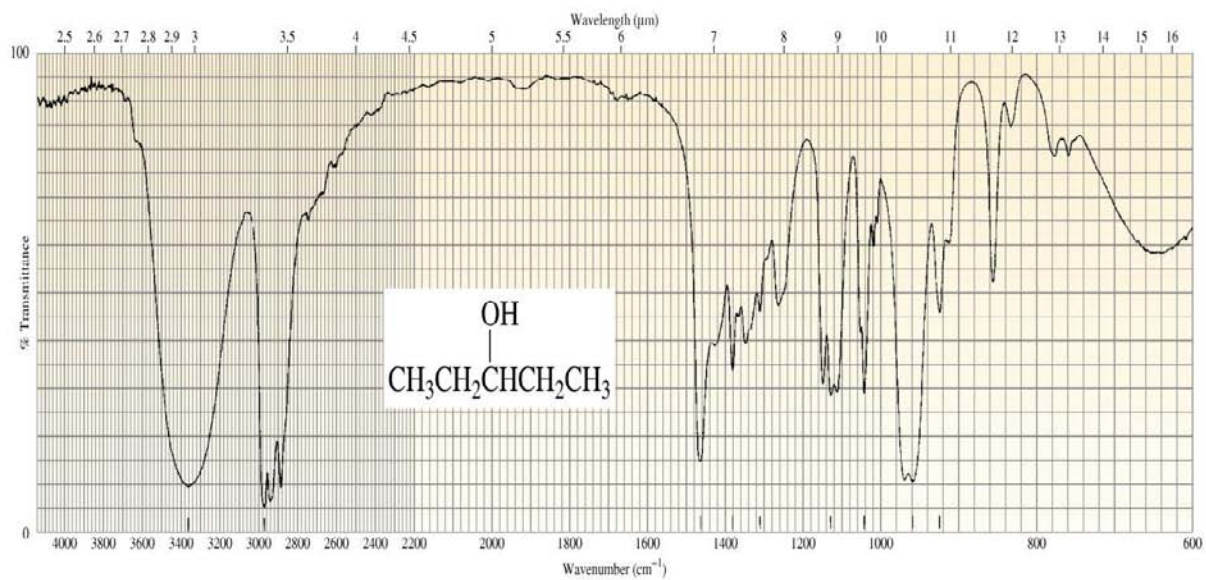


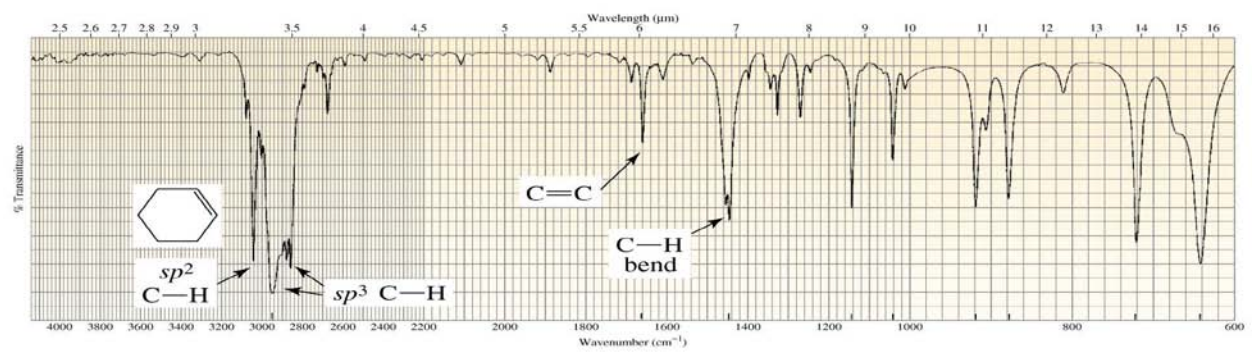
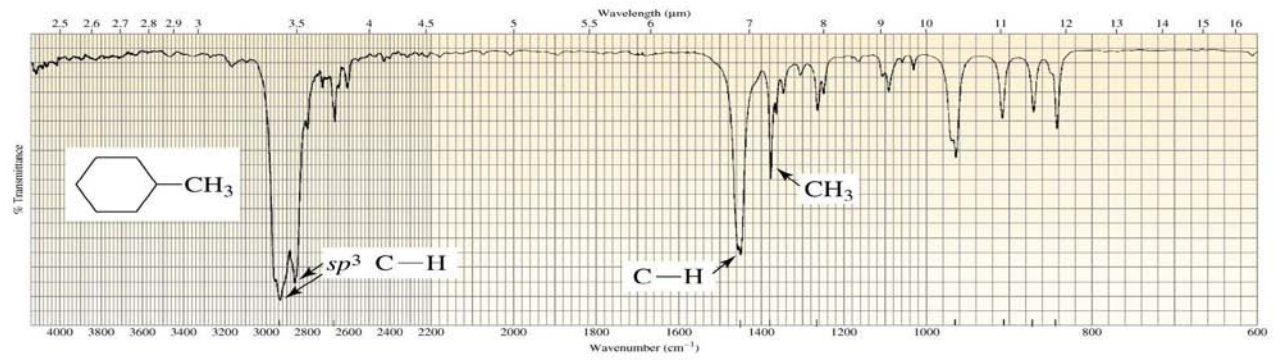
$\tilde{\nu}$ (cm^{-1})	
4000	1000
Functional Group Region	Finger print Region
Stretching	Bending

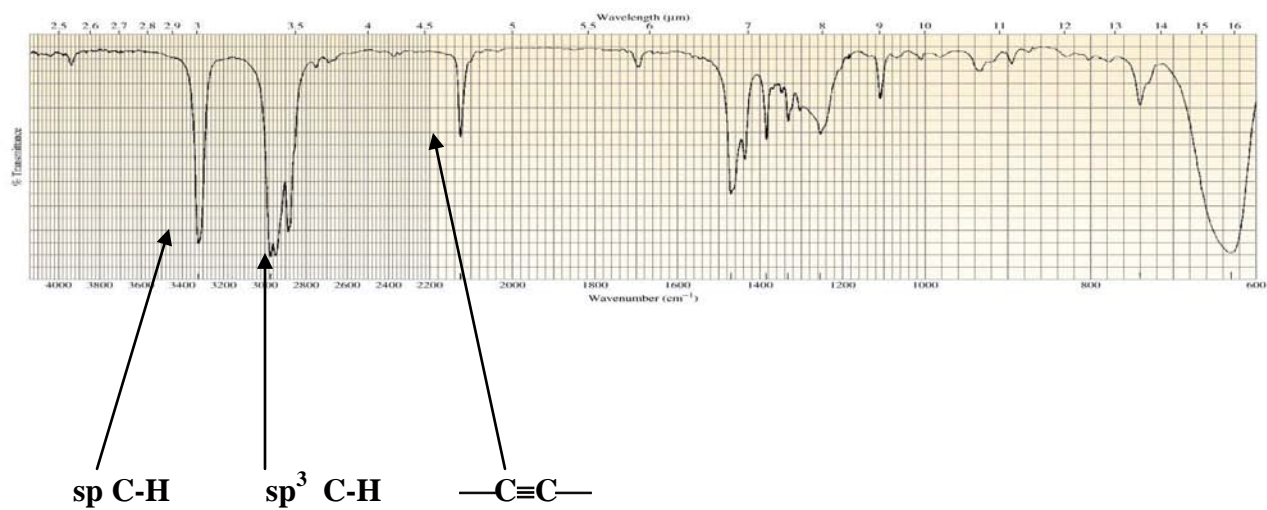
a.



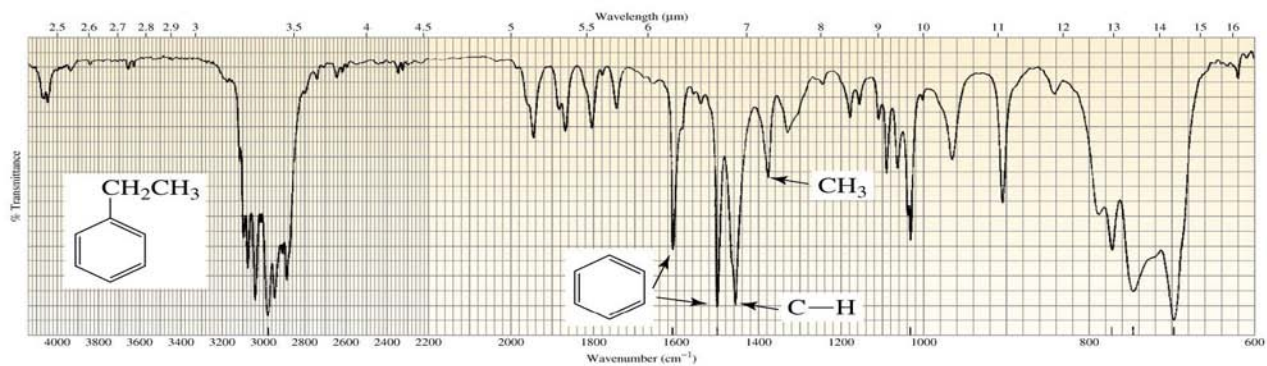
b.

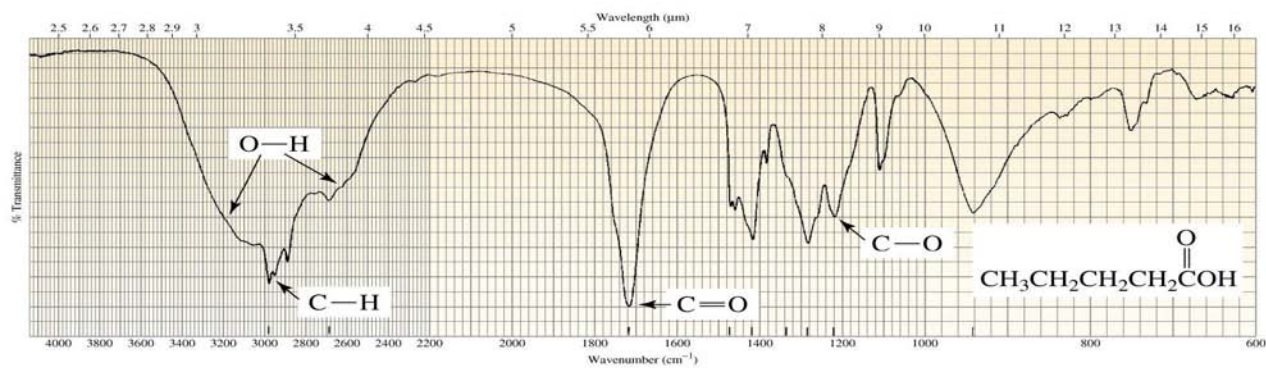
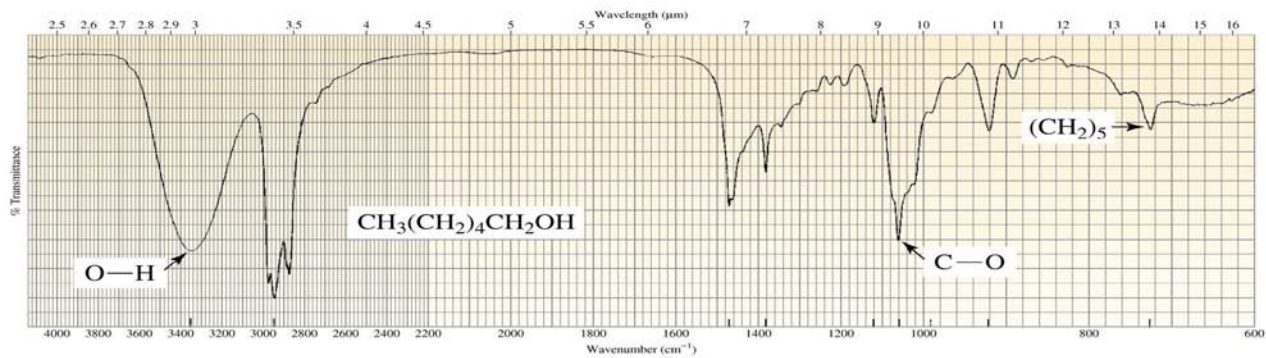


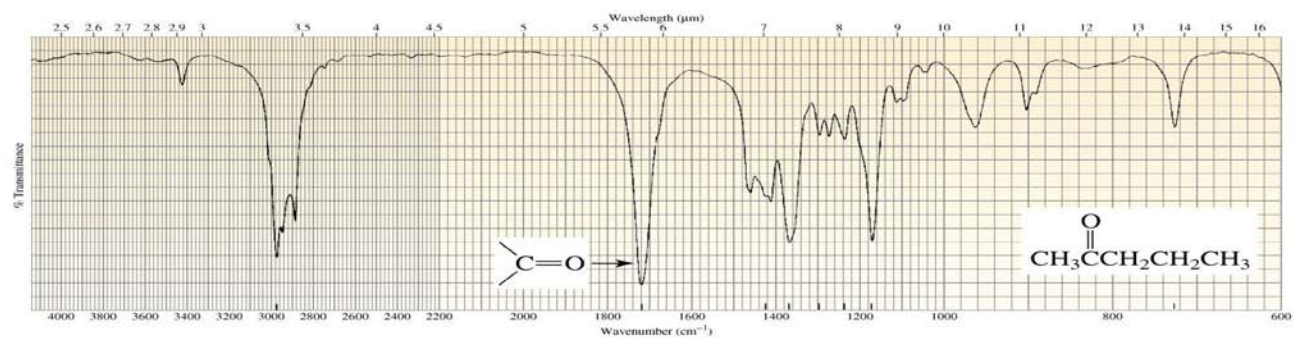
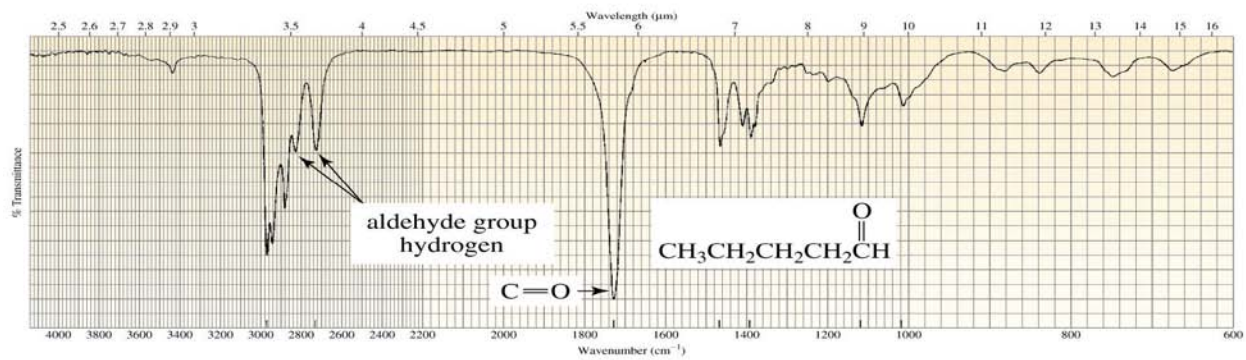


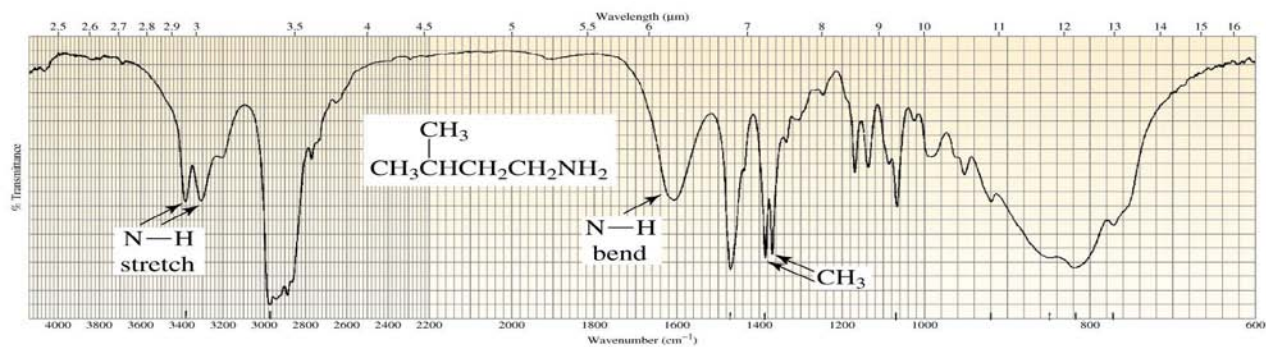
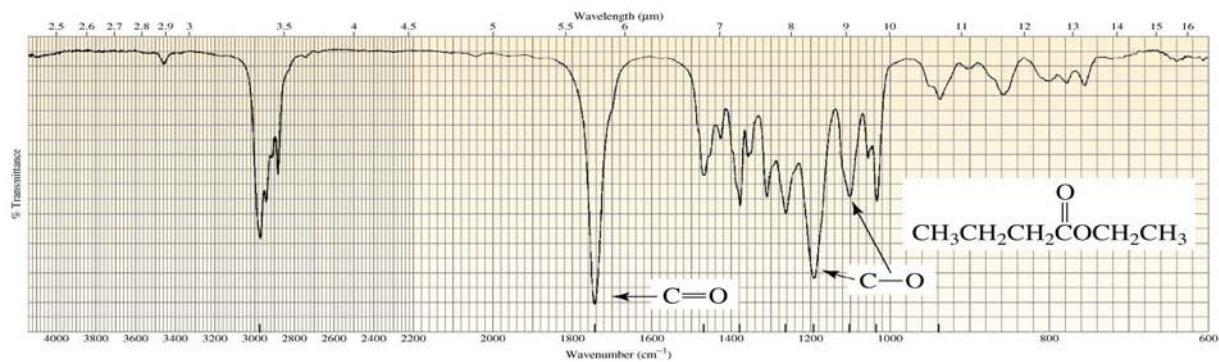


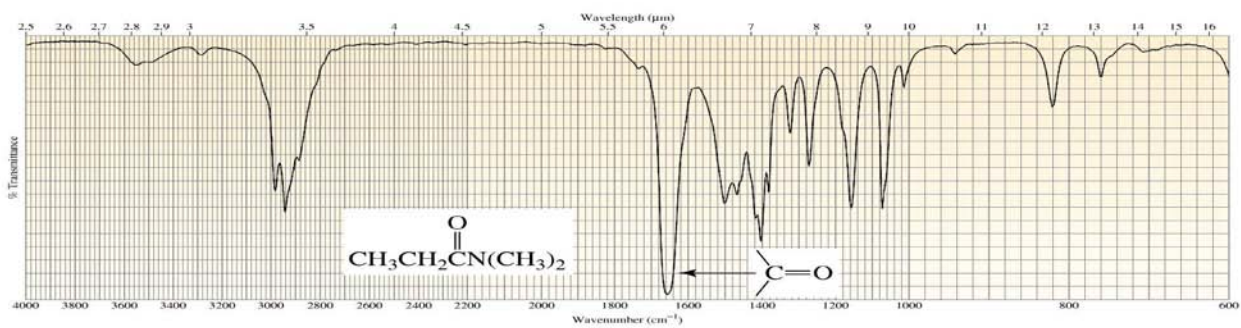
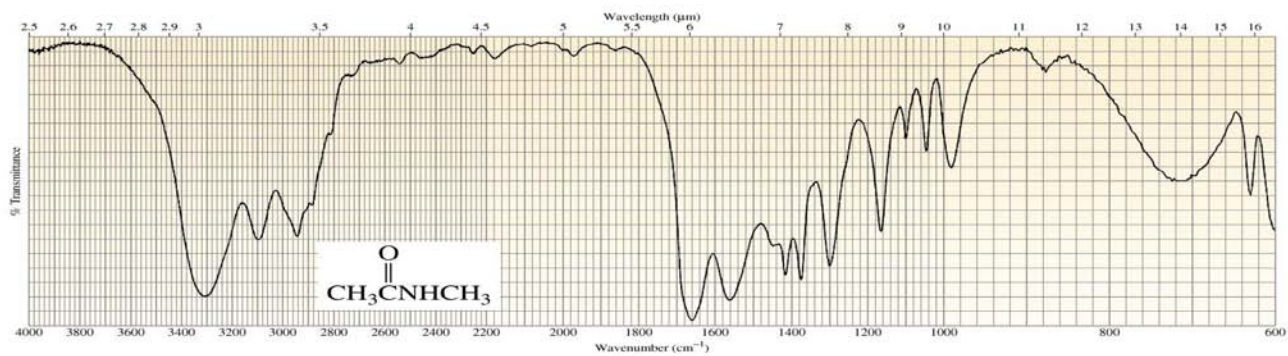
The IR spectrum of CH3CH2CH2CH2C#CH











Infrared Stretching Frequencies

Bond	$\tilde{\nu}$ (cm^{-1})
1. C—H	
a) —C—H	2800-3000
b) =C—H	3000-3100
c) \equiv C—H	3300 (sharp)
2. C—C	
a) C—C	1150-1250
b) C=C	1640-1690
c) C \equiv C	2210-2260
3. C—N	
a) C—N	1030-1230
b) C=N	1600-1690
c) C \equiv N	2210-2260
4. C—O	
a) C—O	1020-1275
b) C=O	1650-1800
5. C—X	
a) C—F	1000-1350
b) C—Cl	800-850
c) C—Br	500-600
d) C—I	200-500
6. N—H	
a) RNH ₂ , RCONH ₂	3400-3500 (two bands)
b) R ₂ NH, RCONHR	3400-3500
7. O—H	
a) ROH	3200-3600
b) RCO ₂ H	2500-3500
8. Aldehyde C—H	2820-2900 (sometimes buried under sp ³ C-H stretch), 2700-277

