



William H. Brown  
Christopher S. Foote  
Brent L. Iverson  
Eric Anslyn

<http://academic.cengage.com/chemistry/brown>

## Chapter 12

# Infrared Spectroscopy

*William H. Brown • Beloit College*

# Molecular Spectroscopy

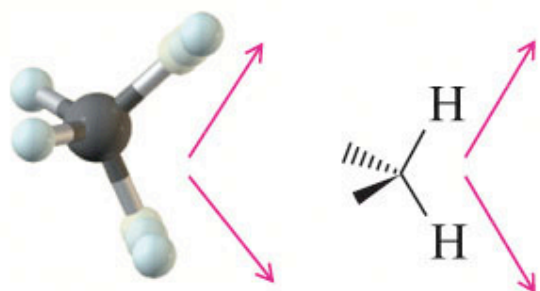
◆ **Molecular spectroscopy** The study of which frequencies of electromagnetic radiation are absorbed or emitted by a particular substance and the correlation of these frequencies with details of molecular structure.

- we study three types of molecular spectroscopy

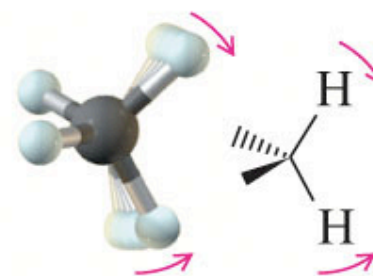
Region of the Electromagnetic Spectrum	Frequency (hetz)	Type of Spectroscopy	Absorption of Electromagnetic Radiation Results in Transition Between
Radio frequency	$3 \times 10^7 - 9 \times 10^8$	Nuclear magnetic resonance	Nuclear spin states
Infrared	$1 \times 10^{13} - 1 \times 10^{14}$	Infrared	Vibrational energy levels
Ultraviolet-visible	$2.5 \times 10^{14} - 1.5 \times 10^{15}$	Ultraviolet-visible	Electronic energy levels

# Molecular vibrations

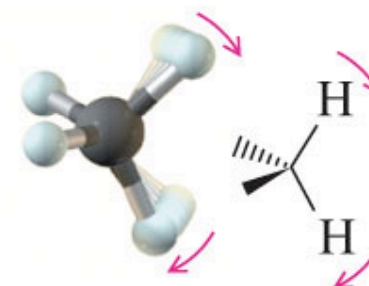
- ◆ Fundamental stretching and bending vibrations for a methylene group.



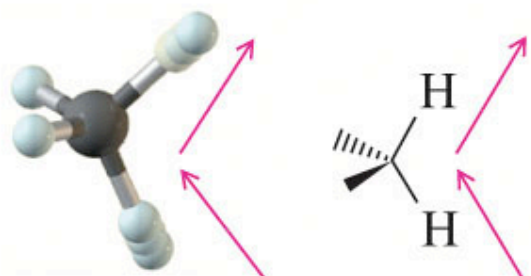
Symmetric stretching



Scissoring

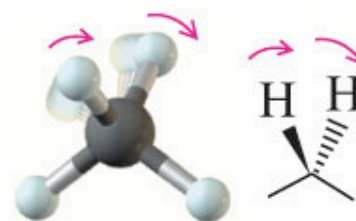


Rocking

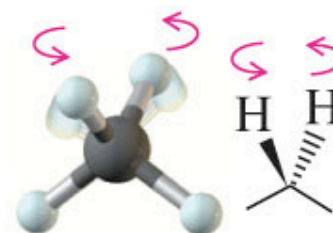


Asymmetric stretching

**Stretching vibrations**



Wagging

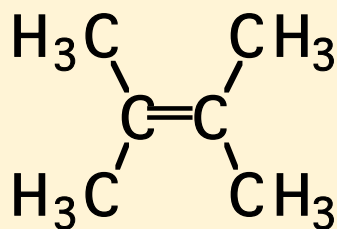


Twisting

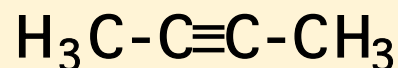
**Bending vibrations**

# Molecular Vibrations

- ◆ **For a molecule to absorb IR radiation**
  - the bond undergoing vibration must be polar and its vibration must cause a periodic change in the bond dipole moment.
- ◆ **Covalent bonds which do not meet these criteria are said to be IR inactive.**
  - The C-C double and triple bonds of symmetrically substituted alkenes and alkynes, for example, are IR inactive because they are not polar bonds.



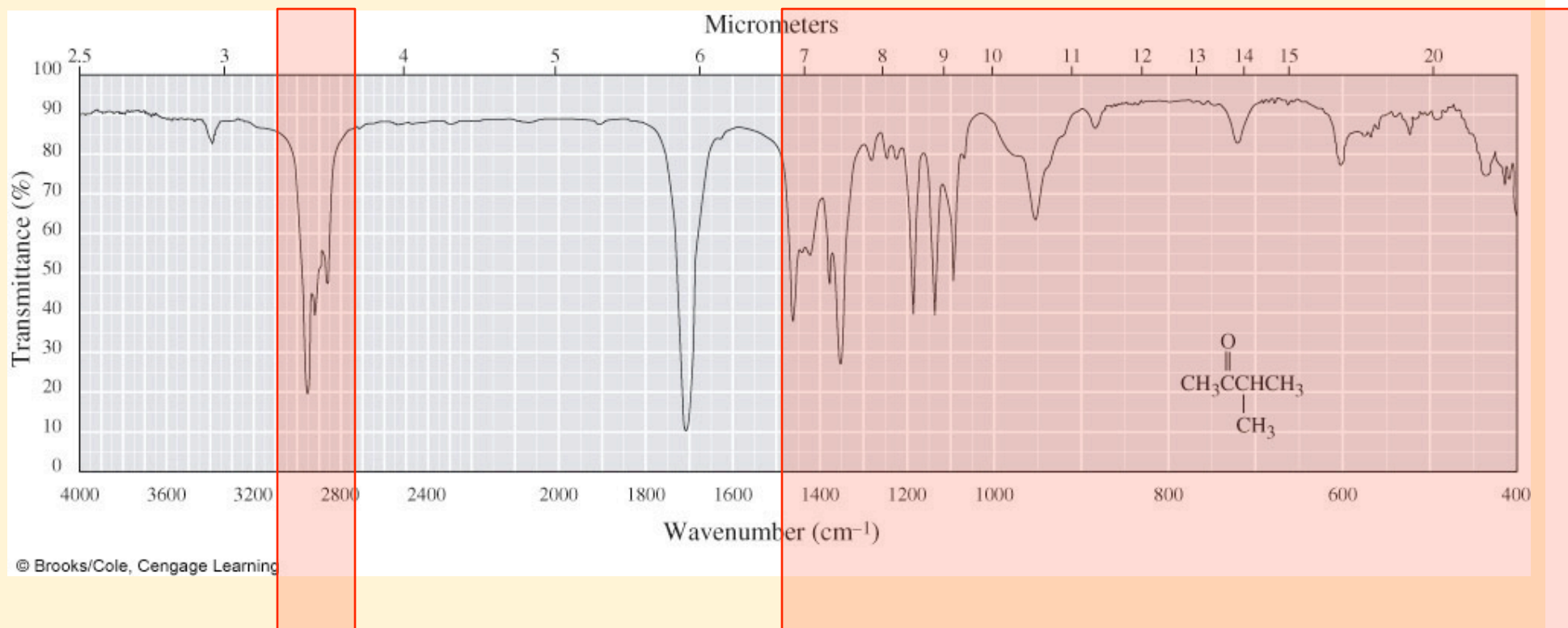
2,3-Dimethyl-2-butene



2-Butyne

# Infrared Spectroscopy

## ◆ Infrared spectrum of 3-methyl-2-butanone.



**C-H Stretching**

**Fingerprint Region:  
Highly Complex and  
Unique for Every Molecule**

# Correlation Tables

## ◆ Infrared stretching frequencies of selected functional groups.

	Stretching		
<u>Less Valuable</u>	Bond	Frequency (cm <sup>-1</sup> )	Intensity
Almost all organic molecules have C-H bonds	O-H	3200-3650	weak to strong
	N-H	3100-3550	medium
C=C often too weak or encroaching on fingerprint region	C-H	2700-3300	weak to medium
	C=C	1600-1680	weak to medium
Buried in fingerprint region	C=O	1630-1820	strong
	C-O	1000-1250	strong

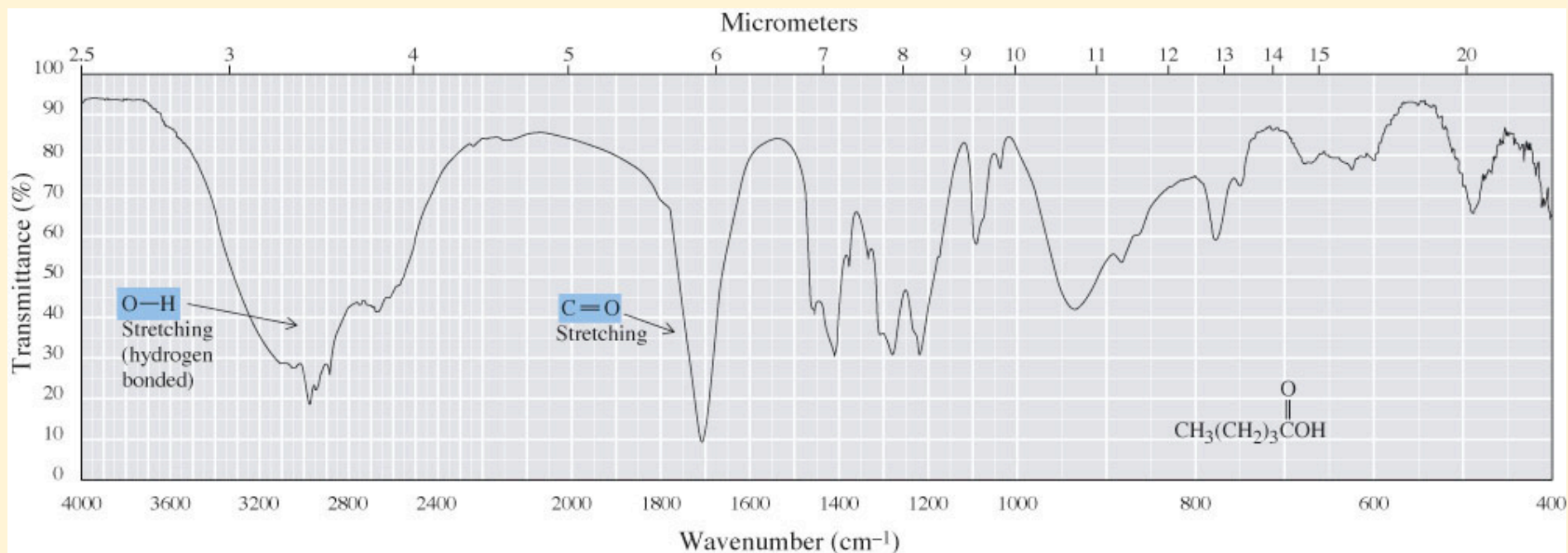
**More Valuable**

Potentially difficult to distinguish between one-another, but good indication of heteroatom-hydrogen bond

Signature Stretch. Very strong, very identifiable

# Carboxylic acids

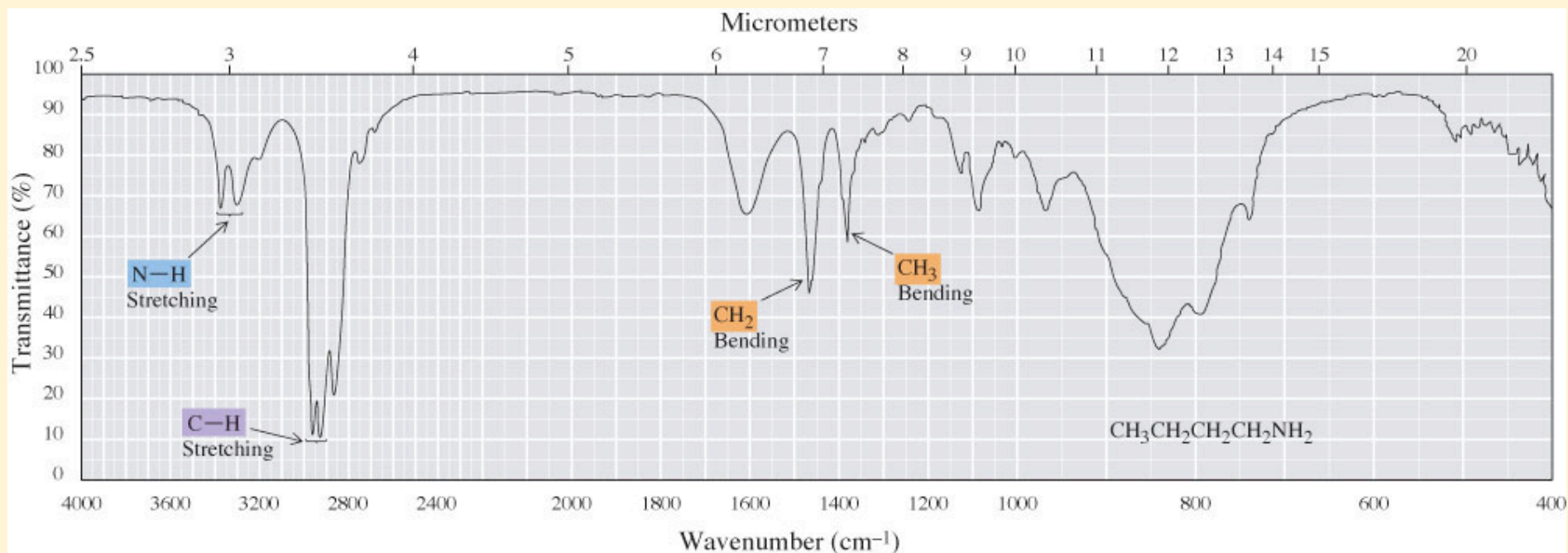
## ◆ Infrared spectrum of pentanoic acid.



© Brooks/Cole, Cengage Learning

# Amines

## ◆ Infrared spectrum of 1-butanamine, a 1° amine.



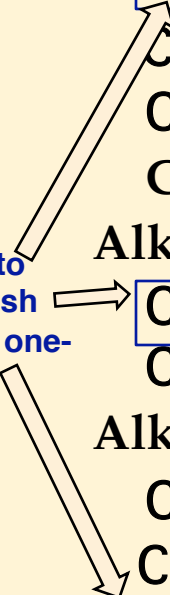
© Brooks/Cole, Cengage Learning



# Hydrocarbons-Table 12.5

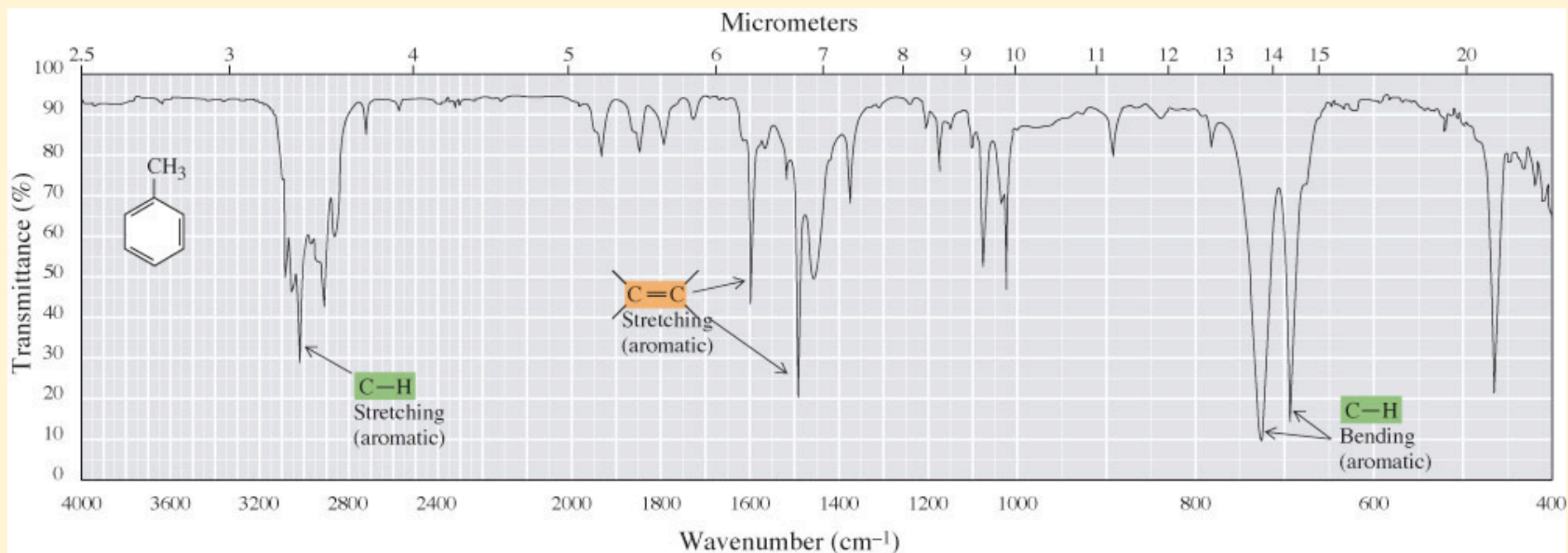
Hydro-carbon	Vibration	Frequency (cm <sup>-1</sup> )	Intensity
<b>Alkane</b>			
C-H	Stretching	2850 - 3000	Medium
CH <sub>2</sub>	Bending	1450-1475	Medium
CH <sub>3</sub>	Bending	1375 and 1450	Weak to medium
C-C	(Not useful for interpretation - too many bands)		
<b>Alkene</b>			
C-H	Stretching	3000 - 3100	Weak to medium
C=C	Stretching	1600 - 1680	Weak to medium
<b>Alkyne</b>			
C-H	Stretching	3300	Medium to strong
C≡C	Stretching	2100-2250	Weak
<b>Arene</b>			
C-H	Stretching	3030	Weak to medium
C=C	Stretching	1450-1600	Medium
C-H	Bending	690-900	Strong

Difficult to distinguish between one-another



# Aromatics

## ◆ Infrared spectrum of toluene.



© Brooks/Cole, Cengage Learning

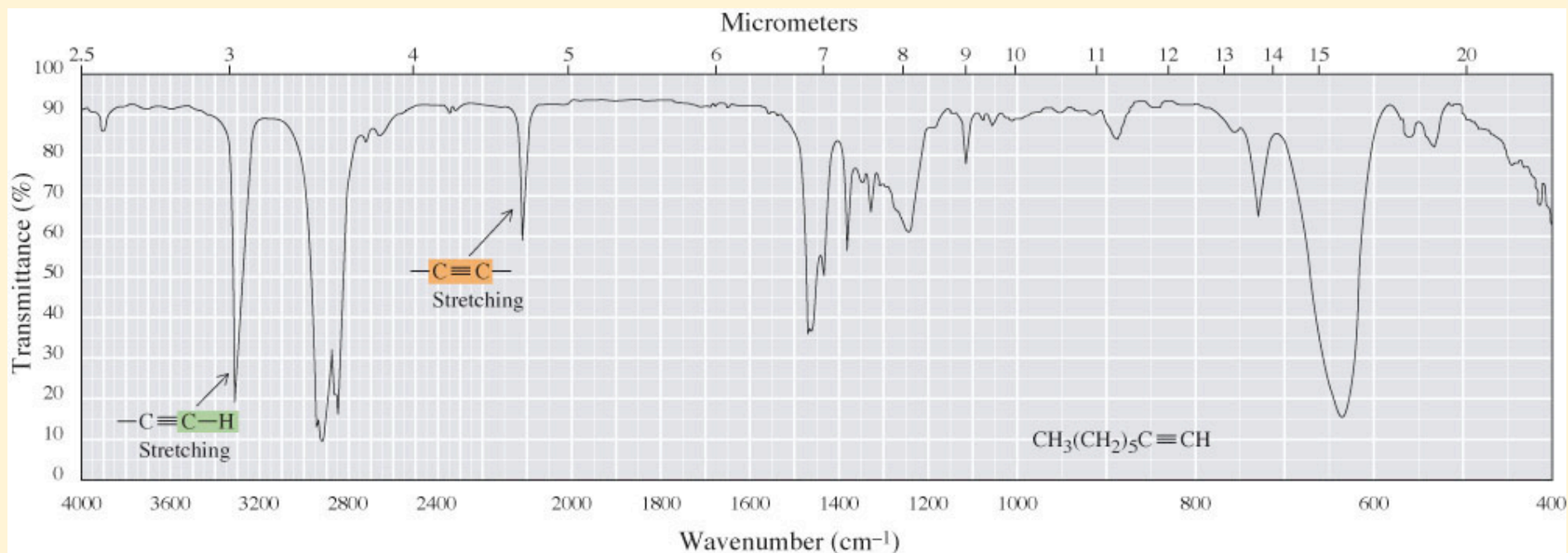
# Hydrocarbons-Table 12.5

Hydro-carbon	Vibration	Frequency (cm <sup>-1</sup> )	Intensity
<b>Alkane</b>			
C-H	Stretching	2850 - 3000	Medium
CH <sub>2</sub>	Bending	1450-1475	Medium
CH <sub>3</sub>	Bending	1375 and 1450	Weak to medium
C-C	(Not useful for interpretation - too many bands)		
<b>Alkene</b>			
C-H	Stretching	3000 - 3100	Weak to medium
C=C	Stretching	1600 - 1680	Weak to medium
<b>Alkyne</b>			
C-H	Stretching	3300	Medium to strong
C≡C	Stretching	2100-2250	Weak
<b>Arene</b>			
C-H	Stretching	3030	Weak to medium
C=C	Stretching	1450-1600	Medium
C-H	Bending	690-900	Strong

Can be useful.  
In fairly distinct  
regions

# Alkynes

## ◆ Infrared spectrum of 1-octyne.



© Brooks/Cole, Cengage Learning