







Region of infrared that is most useful lies between 2.5-16  $\mu$ m (4000-625 cm<sup>-1</sup>)

depends on transitions between vibrational energy states

Stretching: higher energy / higher wave number (cm-1)

Bending: lower energy / lower wave number (cm<sup>-1</sup>)

A bond must have a dipole or an induced dipole in order to have an absorbance in the IR spectrum.

When the bond stretches, the increasing distance between the atoms increases the dipole moment. Therefore, the greater the dipole, the more intense the absorption. (i.e., The greater the molar extinction coefficient ( $\epsilon$ ) in Beer's law, A =  $\epsilon$ bc.

relative polarities relative intensities





## Analyzing Structure: Functions & Infrared Spectra

The molecular formula is a critical piece of information, which limits the functional possibilities.

The presence & absence of absorption bands must be considered in identifying a possible structure in IR spectroscopy. Empiricism is critical to successful identification.

**NOTE:** Bonds which lack dipole moments are not detected.



Important IR Stretching Frequencies			
Type of bond	Wavenumber (cm <sup>-1</sup> )	Intensity	
C≡N	2260-2220	medium	
C≡C	2260-2100	medium to weak	
C=C	1680-1600	medium	
C=N	1650-1550	medium	
$\bigcirc$	~1600 and ~1500-1430	strong to weak	
C=0	1780-1650	strong	
с—о	1250-1050	strong	
C-N	1230-1020	medium	
O—H (alcohol)	3650-3200	strong, broad	
O—H (carboxylic acid)	3300-2500	strong, very broad	
N—H	3500-3300	medium, broad	
С—Н	3300-2700	medium	





Infrared Absorption Frequencies			
Structural unit	Frequency, cm <sup>-1</sup>		
Stretching vibrations (single bonds)			
O—H (alcohols)	3200-3600		
O—H (carboxylic acids)	3000-3100		
N—H	3350-3500		
First examine the absorption bands in the vicinity of 4000-3000 $\mbox{cm}^{-1}$			





Infrared Absorption Frequencies		
Structural unit	Frequency, cm <sup>-1</sup>	
Stretching vibrations (single bonds)		
sp C—H	3310-3320	
sp² C—H	3000-3100	
sp³ C—H	2850-2950	
sp² C—O	1200	
sp <sup>3</sup> C—O	1025-1200	

Infrared Absorption Frequencies		
Structural unit	Frequency, cm <sup>-1</sup>	
Stretching vibrations (single bonds)		
sp C—H	3310-3320	
sp <sup>2</sup> C—H	3000-3100	
sp <sup>3</sup> C—H	2850-2950	
sp <sup>2</sup> C—O	1200	
sp <sup>3</sup> C—O	1025-1200	







Infrared Absorption Frequencies				
Structural unit Frequency, cm <sup>-1</sup> C=O				
Aldehydes and ketones	1710-1750			
Carboxylic acids	1700-1725			
Acid anhydrides	1800-1850 and 1740-1790			
Esters	1730-1750			
Amides	1680-1700			























Infrared Absorption Frequencies			
Structural unit	Frequency, cm <sup>-1</sup>		
Bending vibrations of alkenes			
RCH <sup>==</sup> CH₂	910-990		
$R_2C = CH_2$	890		
cis-RCH=CHR'	665-730		
trans-RCH=CHR'	960-980		
R <sub>2</sub> C=CHR'	790-840		







































