

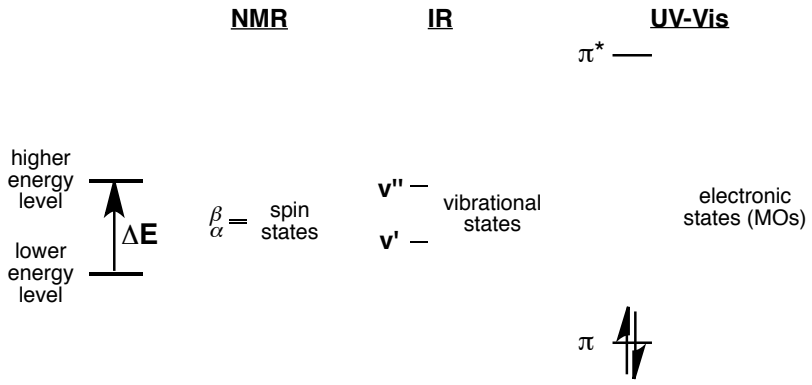
Infrared (IR) Spectroscopy
Learning Objectives

As we study this chapter, you should...

1) Be familiar with the theory behind the technique of infrared (IR) spectroscopy
2) Be familiar with the terminology of IR spectroscopy
3) Be able to interpret an IR spectrum and use it to get clues about the structure and functional groups in an unknown compound
4) Be able to predict the IR spectrum for a compound who's structure is known
5) Be able to predict how structural differences between molecules containing the same functional group will affect its wavenumber of absorbance in an IR spectrum

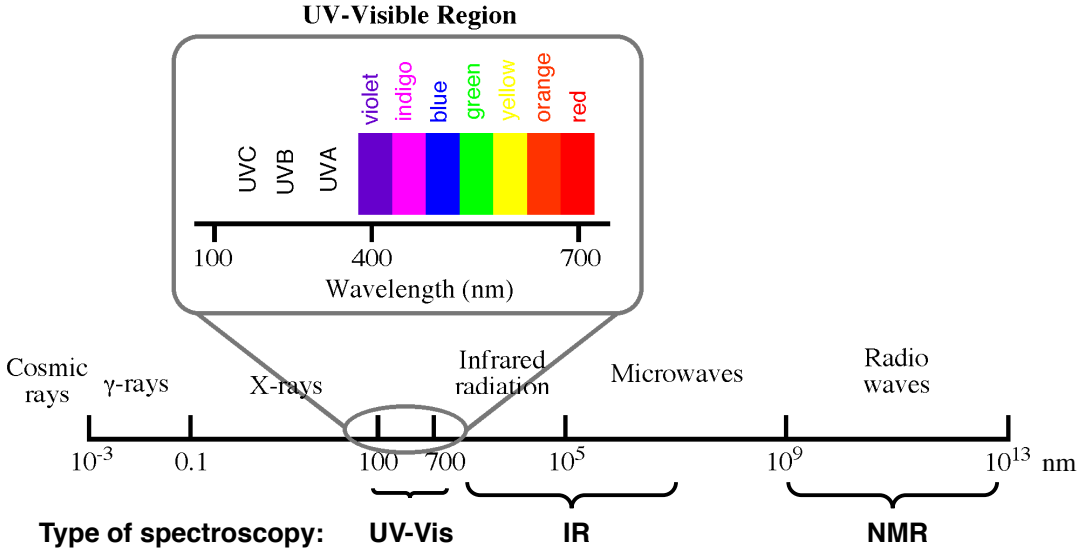
The following concepts and trends are important to Infrared Spectroscopy:

1) **Any technique termed 'absorption *spectroscopy*' involves a transition between different energetic states of a molecule.** The three types of spectroscopy we will encounter and their respective energetic states that are being manipulated are shown*:



*notice the differences in ΔE between the three transitions.

2) **The energy gap between a molecule's different energetic states determines the type of electromagnetic radiation (light) required to effect that transition.**



3) **Infrared (IR) spectroscopy involves transitions between vibrational states of a molecule.** These are the stretching and bending motions that certain parts of a molecule can undergo. In general, stretching transitions take more energy (higher frequency and wavenumbers) than bending transitions. And the stronger/shorter the bond, the more energy is needed to effect a stretching transition. Anything that affects bond strength/length will influence the frequency of light absorbed. *Finally, absorption of energy will only occur if there is a change in dipole in the stretching vibration.*

4) **IR spectroscopy allows us to readily distinguish between various functional groups.** Not only is the position on the x-axis (wavenumbers) important, but the size and shape helps us to determine what functional groups are present based on an IR spectrum... (see next page)

Characteristic IR Absorption Frequencies and Representative Spectra

BOND	FUNCTIONAL GROUP	$\bar{\nu}$ (cm^{-1})
RO–H	alcohols	3200 - 3650
RCO–H	carboxylic acids	2500 - 3300
R_2N–H	amines	3300 - 3500
RC≡C–H	alkynes	3260 - 3330
C=C–H	alkenes	3050 - 3150
–C–H	alkanes	2840 - 3000
RC(=O)–H	aldehydes	2695 - 2830
RC≡CR	alkynes	2100 - 2260
RC≡N	nitriles	2220 - 2260
RCH(=O) , RCR'(=O)	aldehydes, ketones	1690 - 1750
R-C(=O)-OR	esters	1735 - 1750
R-C(=O)-OH	carboxylic acid	1710 - 1760
C=C	alkenes	1620 - 1680
RC–OR'	alcohols, ethers	1000 - 1260