FTIR, and UV-Vis Spectroscopy Techniques

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- Introduction to FTIR
- Theory of FTIR
- Types of Vibration
- Instrumentation
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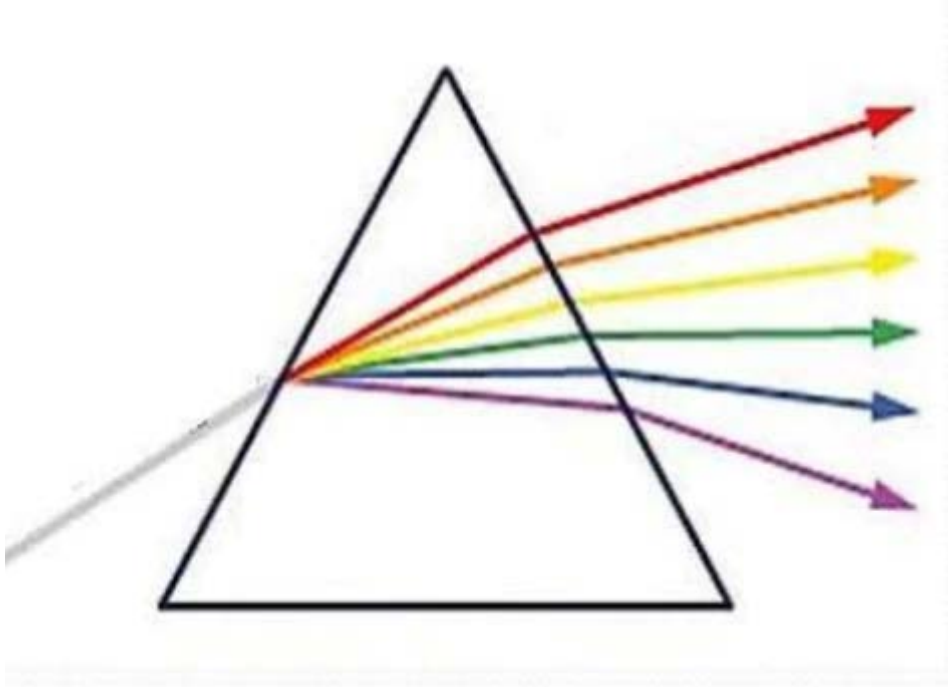
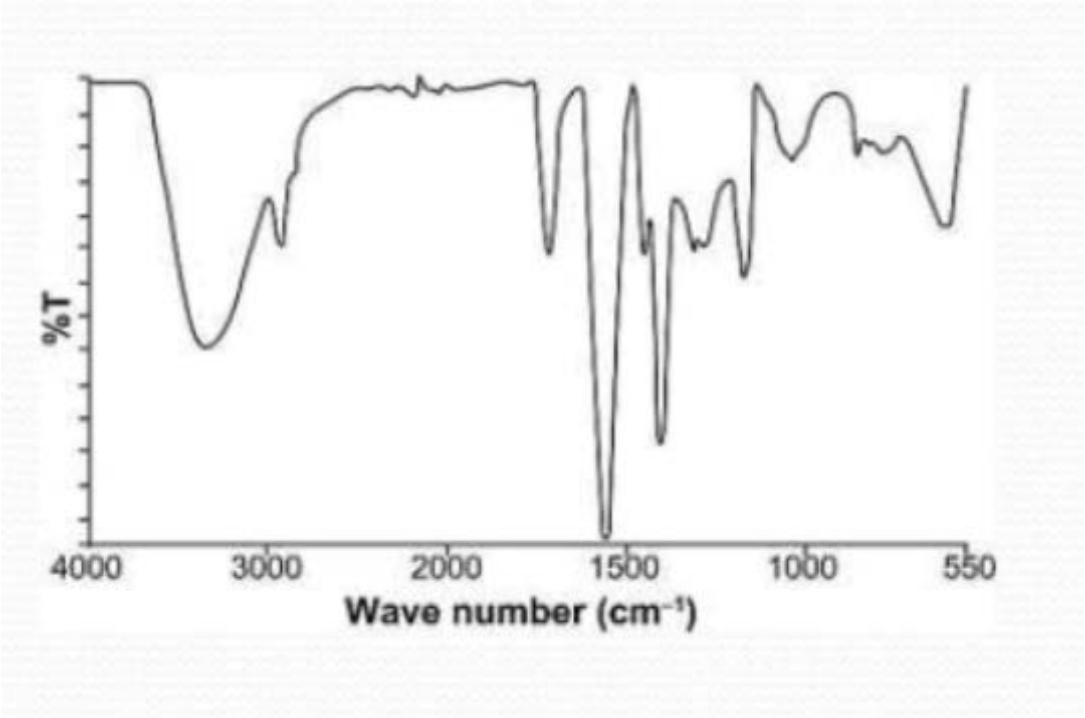
Spectroscopy

Spectroscopy is the science of studying the interaction between radiation and matter



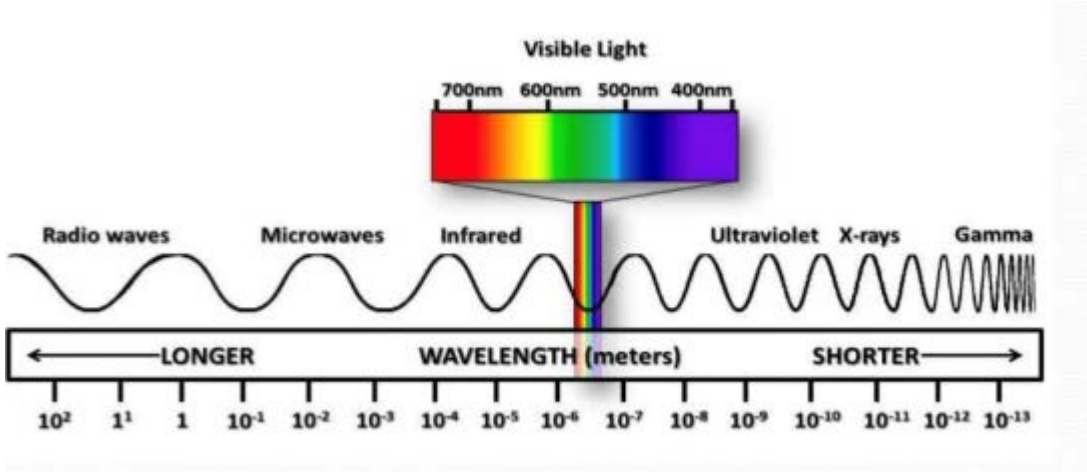
Fourier Transform Infrared

- FTIR Spectroscopy is a molecular spectroscopy which is used to characterize both organic and inorganic information
- The sample is bombarded with infrared radiation
- When the frequency of the infrared radiation matches the natural frequency of the bond, the amplitude of the vibration increases and the infrared is absorbed
- The output of an infrared spectrophotometer is a chart.



Radiation

- Electromagnetic Spectrum: The electric and Magnetic field are oscillating in single planes at the right angle from each other.
- Electromagnetic radiation is the energy propagated through free space or through a material medium in the form of electromagnetic waves.



IR Radiation

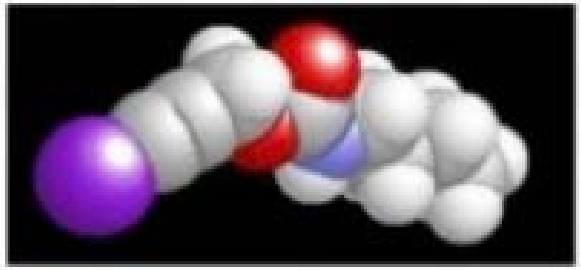
- Electromagnetic radiation at wavelengths longer than the red end of visible light and shorter than microwaves (roughly between 1 and 100 microns).

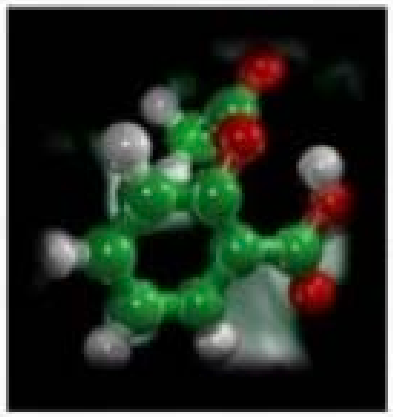
- Our Skin emits infra red light and it’s captured by night vision goggles.

Matter

The Tested Sample

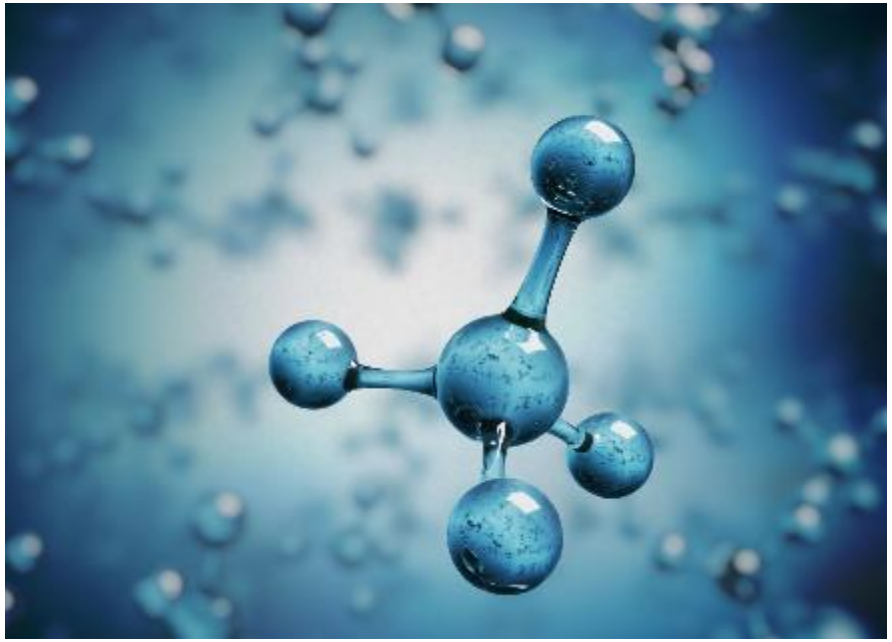
- Polymers, Drugs, Nanomaterials, Nanopowders, Thin films





Interaction of Radiation

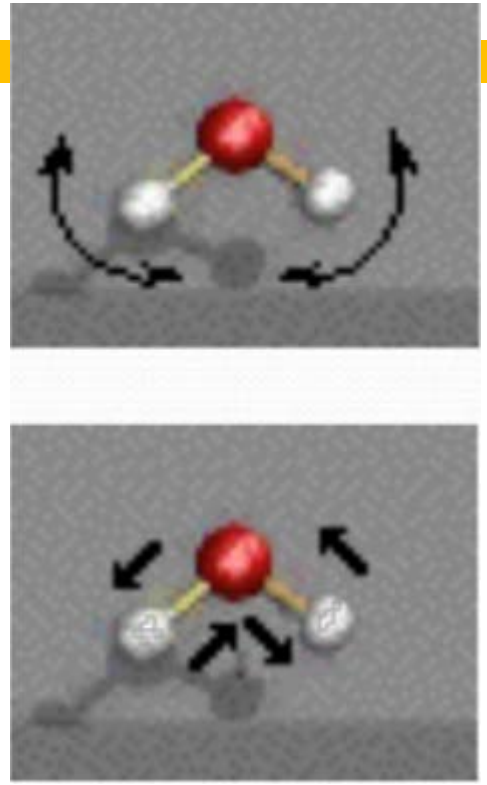
- External energy (excitation energy) can be absorbed only in correspondingly discrete amounts, since the excited states of molecular systems only have certain discrete energy values

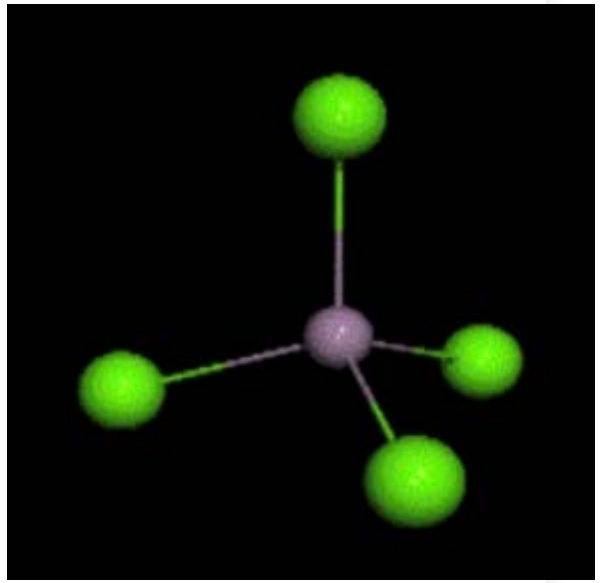


Types of Vibration

- **Stretching:** Change in inter-atomic distance along bond axis. Stretching absorption usually produces stronger peaks than bending

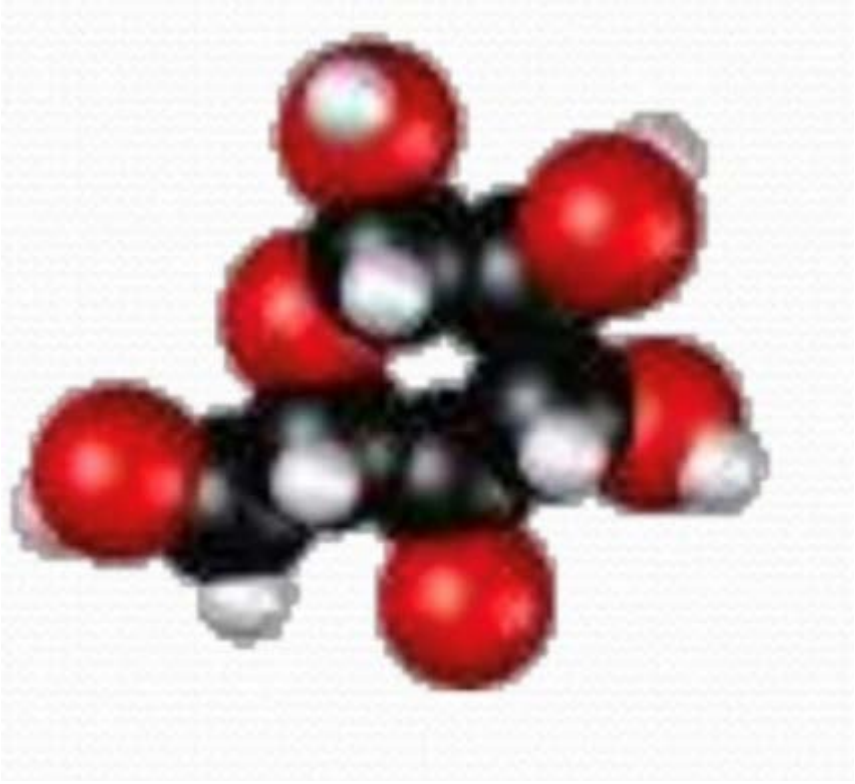
- **Bending** in angle between two bonds
- Scissoring
- Rocking
- Twisting
- Wagging





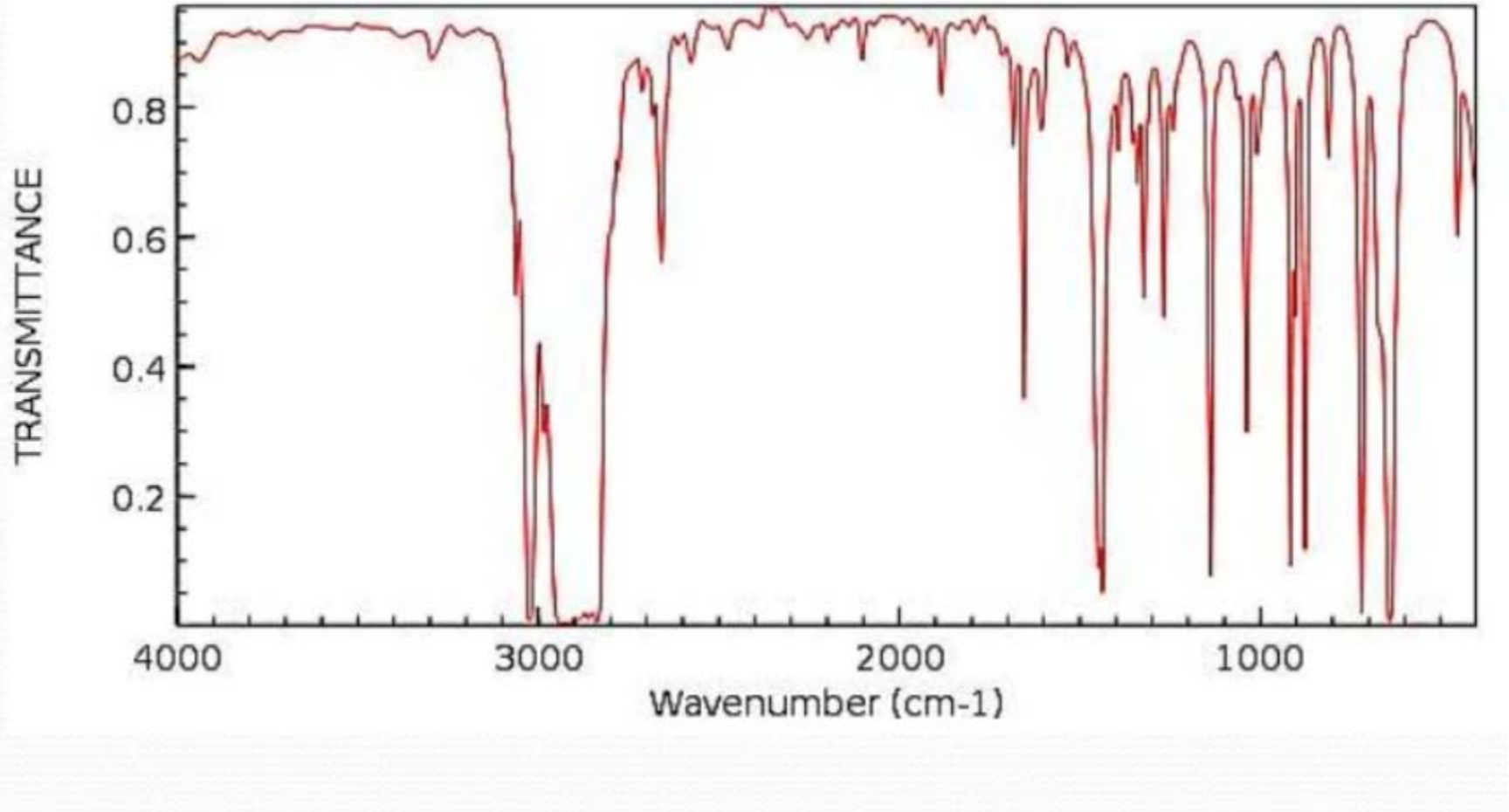
Rotational Motion

- Rotational energy, which gives rise to its own form of spectroscopy, is observed as the tumbling motion of a molecule, which is the result of the absorption energy within the microwave and NIR regions.

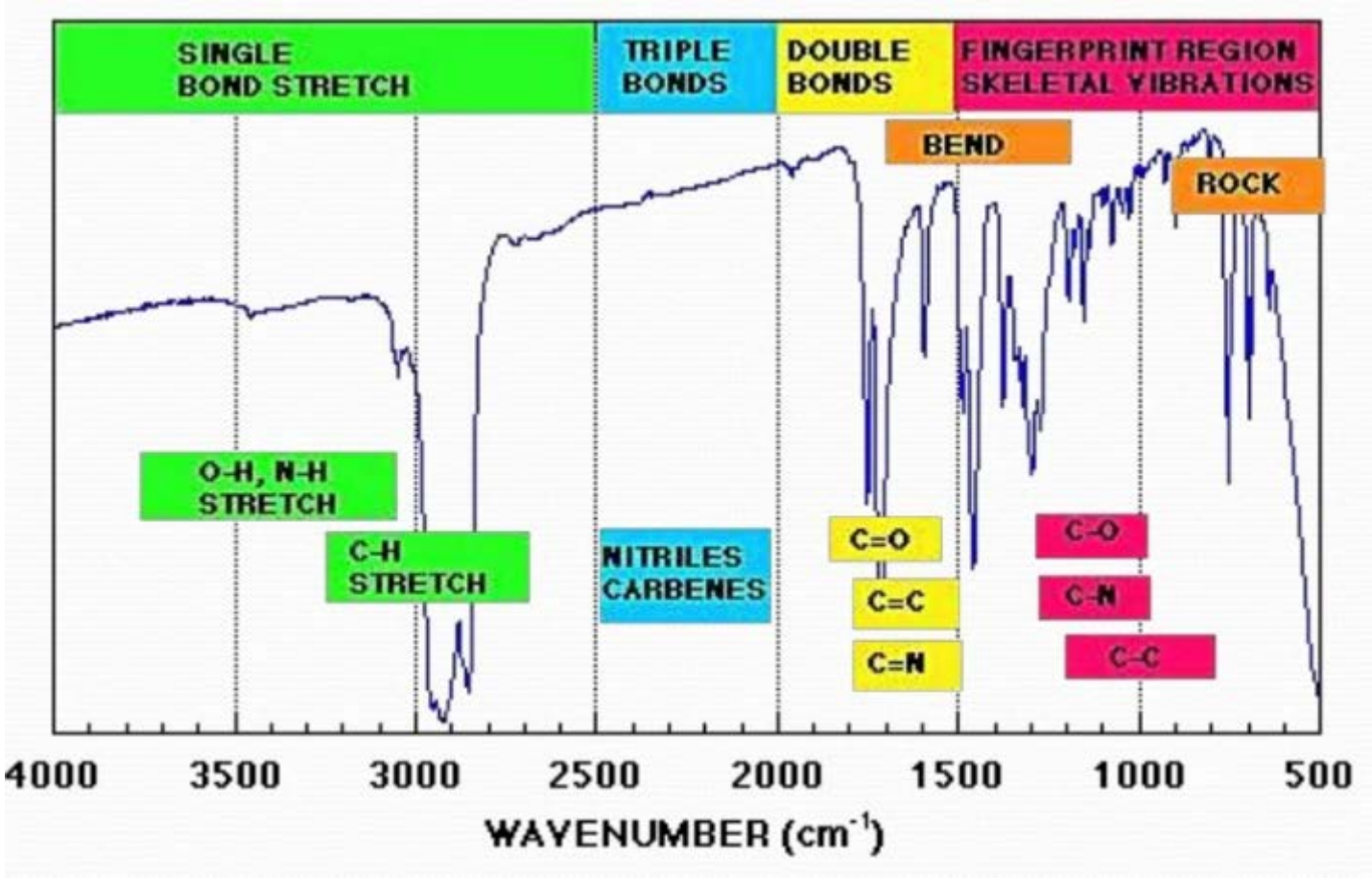


IR Chart

This Chart is a result of interaction between IR radiation and matter

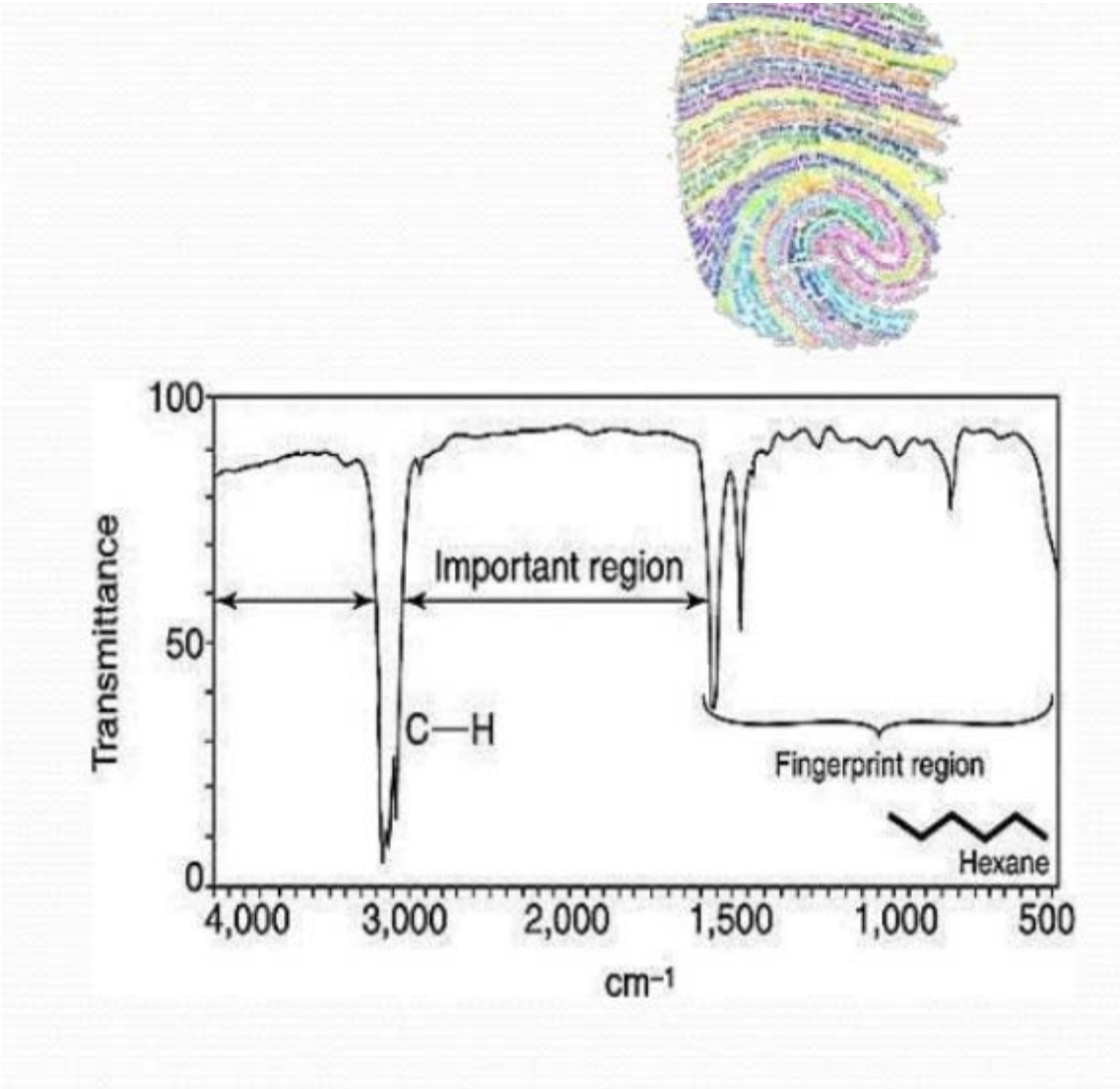


Four Regions of Chart



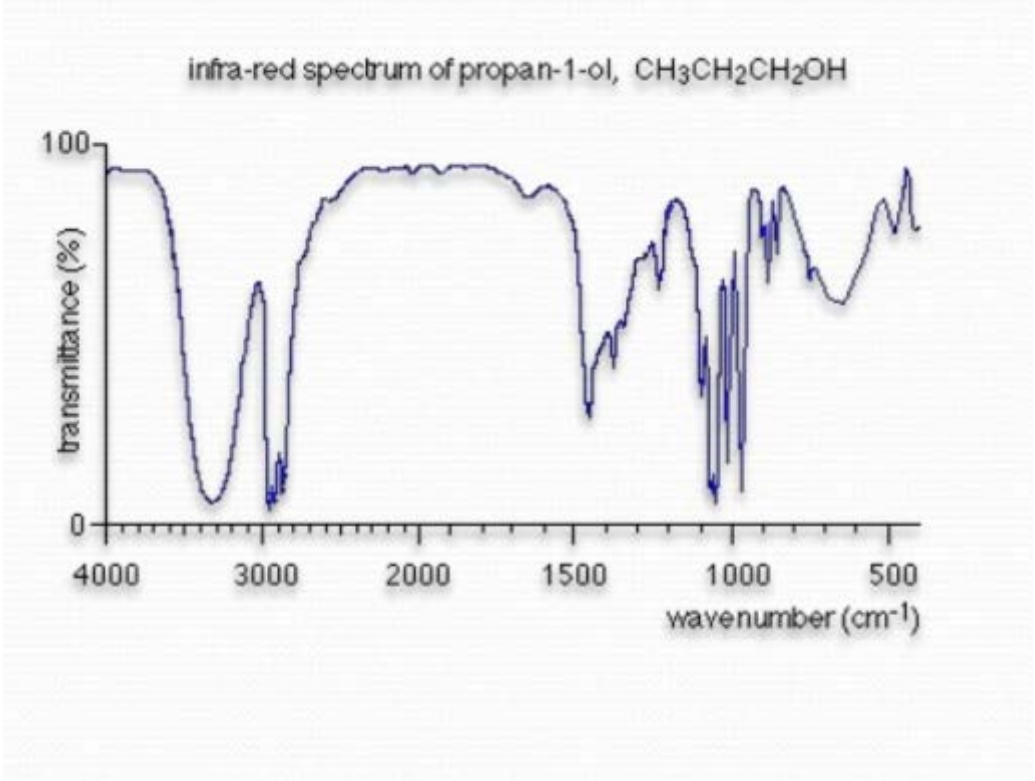
Fingerprint Region

- The region to the right-hand side of the diagram (from about 1650 to 500 cm -1)
- Usually contains a very complicated series of absorption
- Contains peaks due to bending vibration



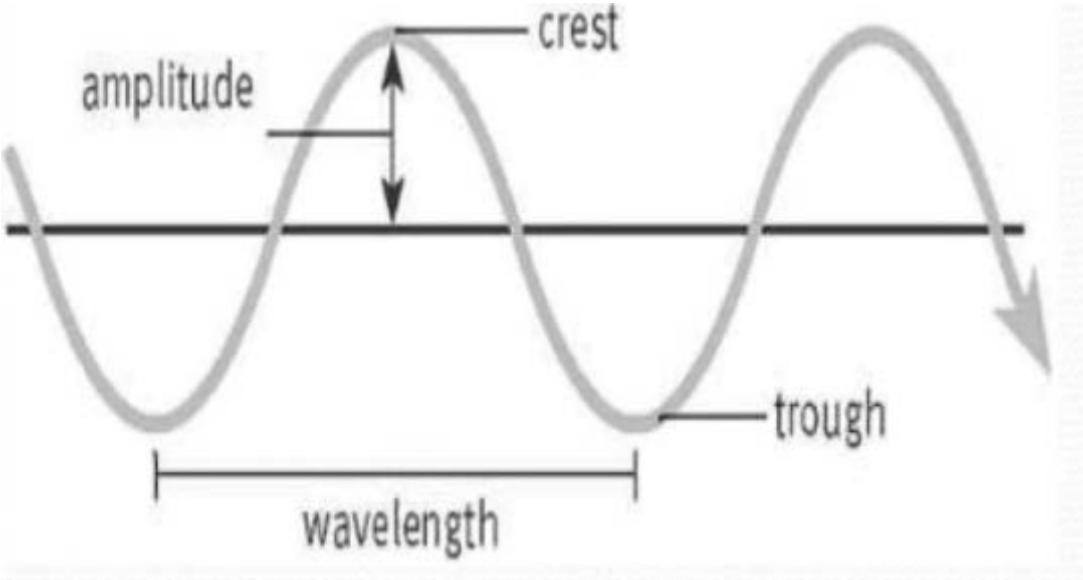
Properties of a Peak

- Intensity (weak, medium or strong)
- Shape (broad or sharp), and
- Position (cm-1) in the spectrum



Definitions

- Wavelength
- The Wavelength is the distance between two identical points of two identical waves in a beam



- Wave number
- Wave number is the number of waves fitting into a unit of distance. The wave number has unit of 1/distance, or distance $^{-1}$. e.g cm $^{-1}$

Working Operation of FITR

- FTIR is used to analyze the functional groups and Chemical bonding in a molecule.
- In FTIR electromagnetic waves in the frequency range of IR is shined though a sample. Based on the certain molecular bonding, the molecule will absorb that energy in specific frequency.
- The absorbed energy will cause the bonds to stretch, bend or rotate.
- The stretching vibration is similar to the oscillation of a spring.

Working Operation of FITR

- As the matter is absorbing energy the, the IR waves at certain frequency are absorbed by the compound, and therefore the transmission of the wave will be less than 100 %.
- We will then have a peak on the FTIR chart. The peaks corresponds to specific chemical bonding and can be used to analyze the chemical bonding and functional group of a matter.

Ultraviolet (UV) and Visible Spectroscopy

- Ultraviolet and visible (UV-Vis) absorption spectroscopy is the measurement of the a beam of light after it passes through a sample or after reflection from a sample surface. Absorption measurements can be at a single wavelength or over and extended spectral range.

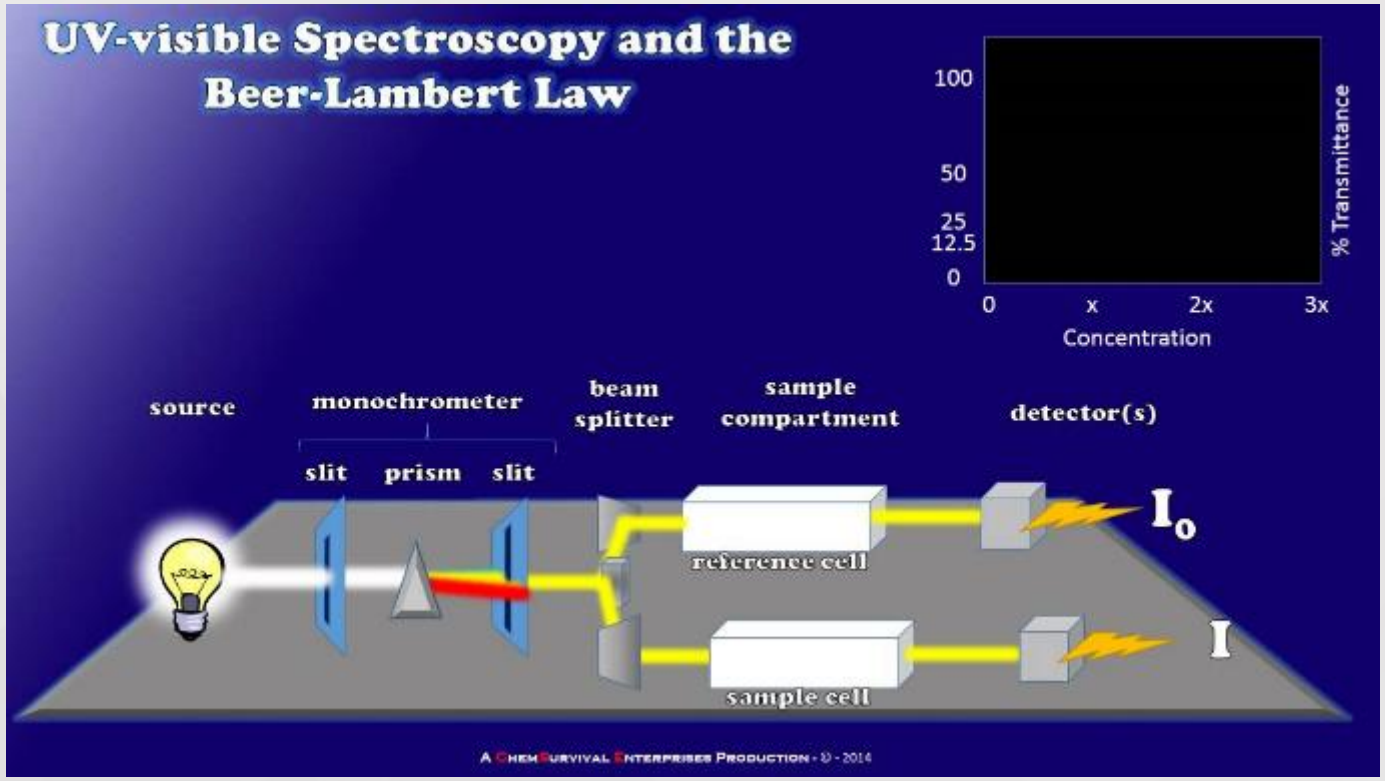
Why we use UV-Vis spectroscopy?

- Analyzing the concentration of matter in solution
- Maximum absorption wavelength
- Detection of functional groups

UV Radiation

- The region beyond red is called infra-red while that beyond violet is called as ultra-violet. The wavelength range of UV radiation starts at blue end of visible light and end at 2000 A.

Ultraviolet absorption spectra arise from transition of electron with in a molecule from a lower level to a higher level.

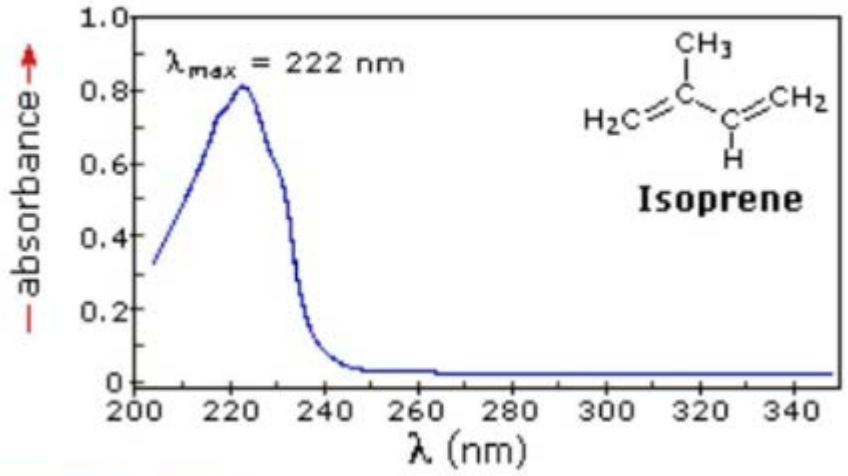


The absorption Spectrum

- When a sample is exposed to light that matches the electronic transition within the molecules fraction of the light energy is absorbed by the molecule and the electrons would be promoted to higher energy state orbital. The UV-VIS spectrometer records the degree of absorption by the sample at different wavelengths and the resulting plot for absorbance versus wavelength is known as a spectrum.

UV Spectrum of Different samples

- UV-visible spectrum of isoprene showing maximum absorption at 222 nm.



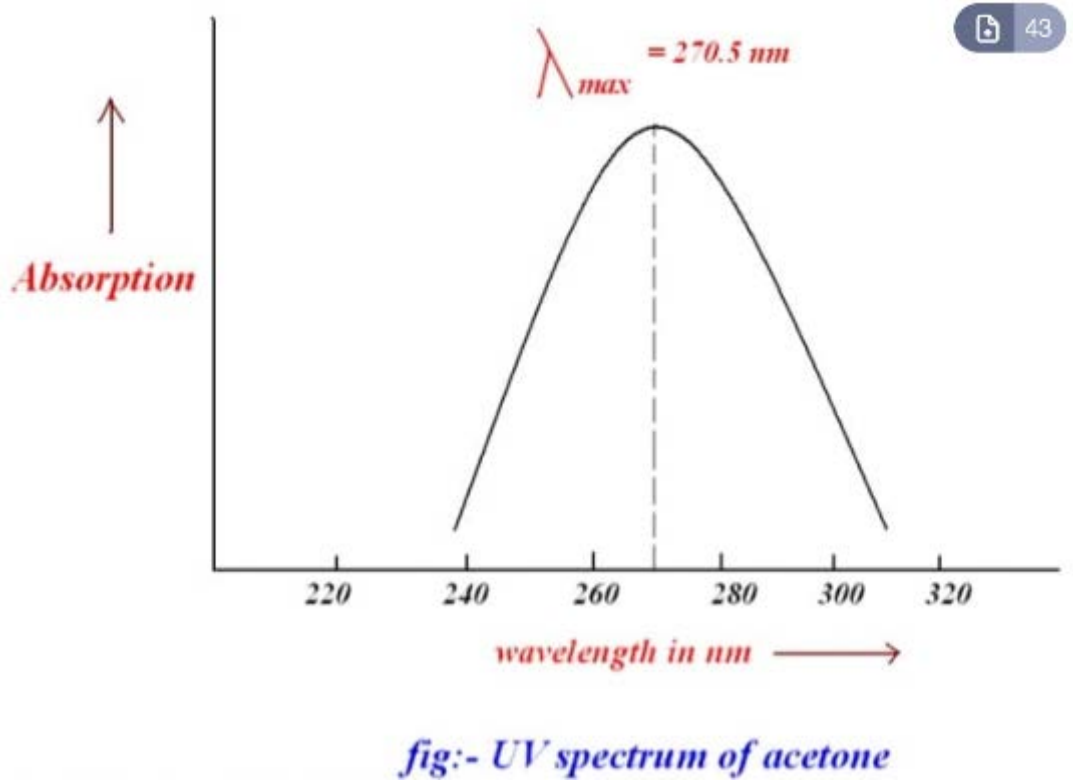


fig:- UV spectrum of acetone

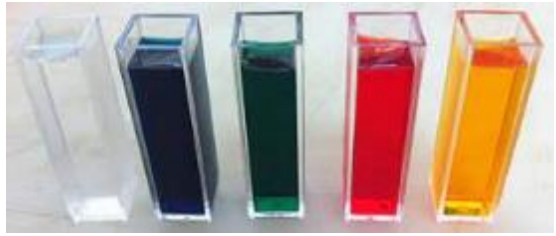
Significant features:

- $\lambda\ max$ (wavelength at which there is a maximum absorption)
- The intensity of max absorption

- The instrument measures Transmittance $\frac{Initial\ intensity\ I0}{Intensity}$
- The transmittance data is then plotted to absorbance (*Abs)*
- Lambert Law : “Absorbance of a light is directly proportional to the path length and the concentration of the absorbing species”

$$A = \varepsilon c l$$

A	Absorbance	
ε	Molar absorption coefficient	$M^{-1}cm^{-1}$
c	Molar concentration	M
l	optical path length	cm



Measurements with UV-Vis

- The intensity of absorbance can be plotted to concentration
- Information on chemical groups