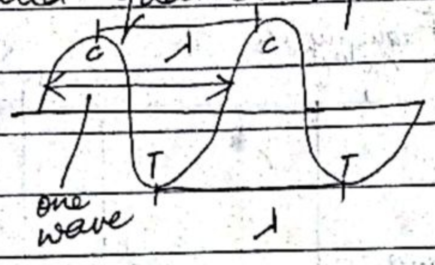
Spectroscopy

Organic chemists use Spectroscopy as a necessary tool for structure determination. Spectroscopy may be defined as the study of the quantized interaction of electromagnetic radiations with matter.

Electromagnetic radiations are produced by the oscillation of electric charge and magnetic field residing on the atom.

Electromagnetic radiation can be described as a wave occuring simultaneously in electrical and magnetic fields and it can also be described as if it consisted of particles called quanta or photons.



The distance between consecutive crests (or troughs) is the wavelength

Electromagnetic radiation is energy. When a molecule absorbs radiation, it gains energy and on emitting radiation, it losses energy. The emission or absorption of electromagnetic radiation is quantized and each quantum of radiation is called a quantum or photon. Energy E for a single photon

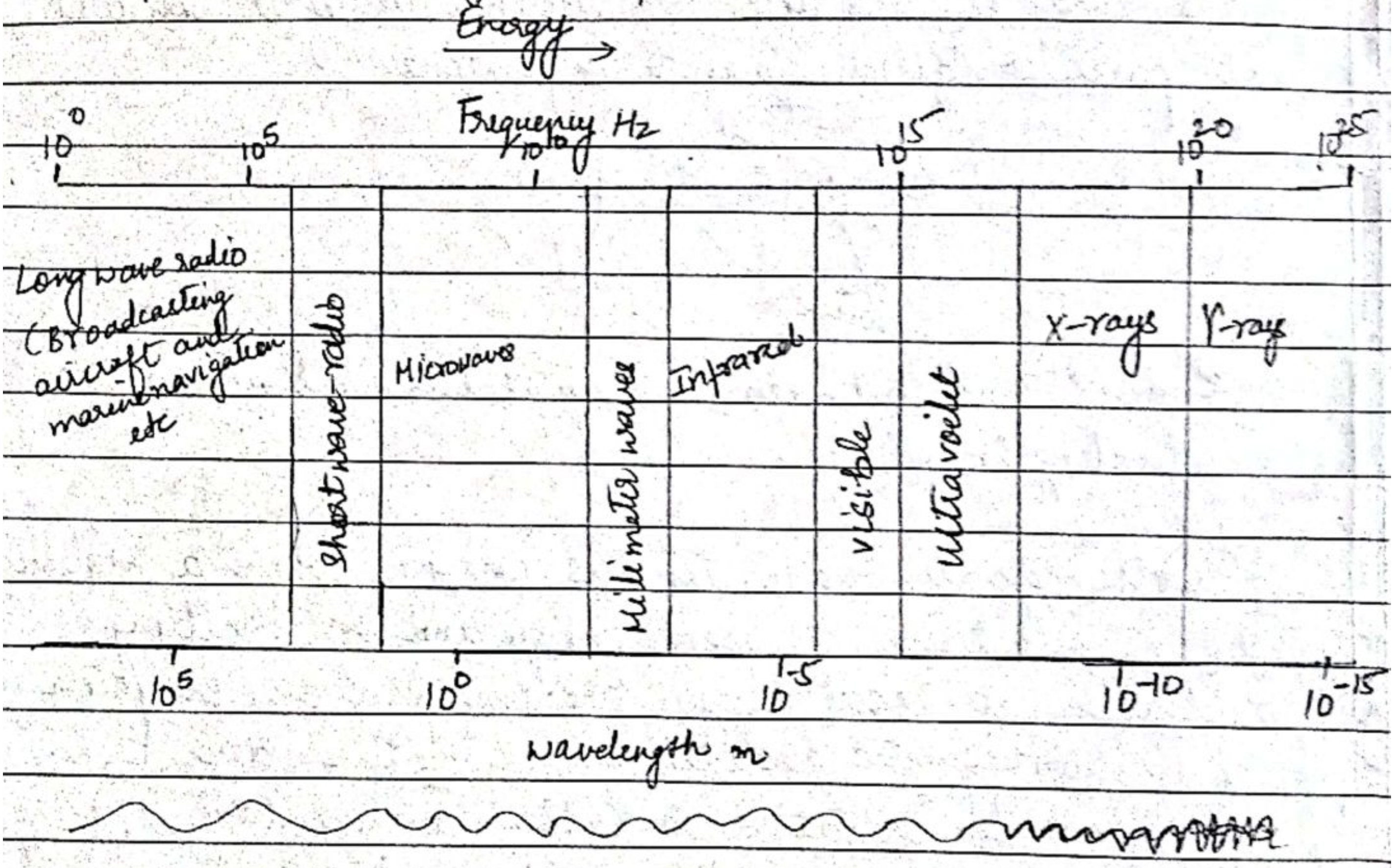
$$E = h\nu = \frac{hc}{\lambda}$$

h = planck's constant

The higher the frequency (or shorter the wavelength) of the radiation, the greater is its energy.

There are various forms of electromagnetic radiation, e.g. light (visible), ultravoilet, infrared, X-rays, microwaves, radiowaves, Cosmic rays etc

Electromagnetic spectrum covers a very wide range of electromagnetic radiations from Cosmic rays to radiowaves at the other end. The arrangement of all types of electromagnetic radiations in order of their wavelength or frequencies is known as Complete electromagnetic Spectrum.



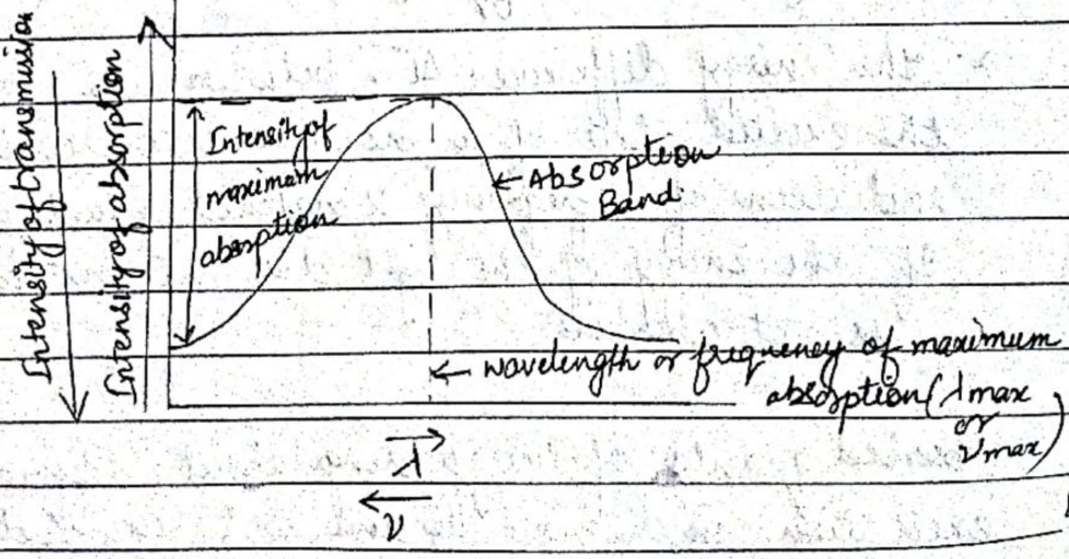
Spectroscopy gives us plenty of information, from Spectra ∴ we can find out

① Bond Order
② Bond Distance
③ Calculate the ratio of different Compound in mixture.
④ Find out purity of Compound
⑤ Isotopic Abundance

DATE

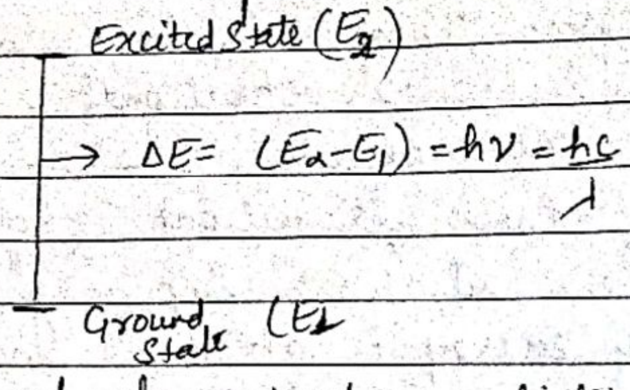
(6) Presence of different functional groups
(7) To find progress of reaction
(8) presence of different atoms (exact mol wt, mass)

When ~~an~~ electromagnetic radiations are passed through an Organic Compound, they may be absorbed to induce electronic, vibrational and rotational transitions in the molecules. The energy required for each of these transitions is quantized. Thus only the radiations supplying the required quantum of energy is absorbed and remaining portion of incident radiation is transmitted. Generally a Spectrophotometer records an absorption spectrum as a plot of the intensity absorbed or transmitted radiations versus their wavelengths or frequencies. Such Spectra which are obtained by absorption of electromagnetic radiations are called absorption Spectra. U.V, Visible, IR and NMR Spectra are examples of absorption Spectra.



The spectra which are obtained by emission of electromagnetic radiations from the excited Substances are known as emission Spectra, like atomic emission

The excitation is caused by heating the substance to a high temperature either thermally or electrically. The excited substance emits certain radiations when it comes to ground state and a spectrometer records these radiations as an emission spectrum.



* Organic molecules absorb radiation in discrete packets of $\Delta E = h\nu$ which are also called quanta of energy
* The energy transition $E_1 \rightarrow E_2$ correspond to absorption of energy exactly equivalent to the energy of wavelength absorbed.
* A molecule can only absorb only a particular frequency if there exist within the molecule an energy transition of magnitude $\Delta E = h\nu$

or

* The energy difference ΔE, between the ground and the excited state of a molecule is overcome by incident radiation of frequency ν matched exactly equal to ΔE. If the energy of the light does not match, then the light is not absorbed

Absorbed quanta of energy bring about different kinds of excitation in a molecule and each require its own distinctive energy, ΔE i.e., Each type of excitation (motion) corresponds to absorption of light in different region of EM Spectrum.

DATE

UltraVoilet (UV) & Visible Spectroscopy

* UV and visible spectroscopy (electronic Spectroscopy) is primarily used to measure bond or aromatic Conjugation
* UV/vis Spectroscopy requires electromagnetic radiation of high energy
* The visible region Correspondings to 800-400 nm and Ultravoilet region to 400-200nm

It is subdivided into near UV region (200-400mm) and the far or vacuum UV region (100-200nm). The visible region extends from 400 to 800nm.

The absorption of electromagnetic radiations in the UV and visible regions induces the excitation of an electron from lower to higher molecular Orbital (electronic energy level). Since UV and visible Spectroscopy involves electronic transitions, it is often Called electronic Spectroscopy

A UV- visible spectrophotometer records a UV or visible Spectrum as a plot of wavelengths of absorbed radiations versus the intensity of absorbtions in terms of absorbance A or molar absorptivity (molar extinction Cofficient) ϵ as defined by Lambert-Beer Law.

$$\log_{10} \frac{I_0}{I} = A = \epsilon c l$$

I_0 = Intensity of incident radiation
I = Intensity of transmitted radiation
C = Concentration of Solute (mole/litre)
l = path length of Sample (cm)

The molar absorptivety of an Organic Compound is Constant at given wavelength and is reported as ϵ_{max} — the molar absorptivity at maximum absorption. The wavelength of the maximum absorption is denoted by λ_{max}