Spectroscopy:-

Transitions that a molecule undergoes between its energy levels upon absorption of suitable radiations determined by quantum mechanical selection rules.

Quantum mechanics tells that the energy levels of all systems are quantized and are designated by appropriate quantum numbers.

These energy levels are obtained by the solutions of the time - independent Schrodinger equation, the details of which are not really essential to the understanding of spectroscopy.

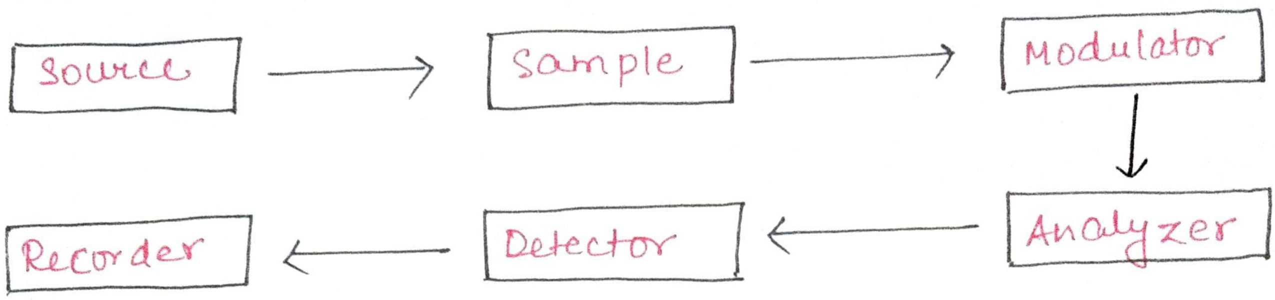
Let us consider how a spectrum arises.

(a) Absorption spectrum (b) Emission spectrum.

- Em and En are two energy levels
- A photon of frequency ν falls on the molecule in the ground state and its energy hν is exactly equal to the energy differences $\Delta E (= E_m - E_n)$ between two molecular energy levels.
- The molecule undergoes a transition from lower to higher energy level with absorption of energy (hν). This called Absorption band.

- If the molecule falls from the excited state of to the ground state with the emission of photon of emission of a photon of energy $h\nu$. The spectrum is called emission spectrum.

Basic Features of Spectrometer:



schematic representation of absorption spectroscopy

The basic set up of IR and UV-Vis regions of electromagnetic spectrum.

→ **Source**:- The source produces radiation spanning a range of frequencies, but in a few cases (such as lasers), it is almost monochromatic radiation.
The radiation source in an absorption spectrometer is a heated ceramic filament coated with rare-earth oxides – Nernst emitter or filament for IR region.
For visible region of spectrum is a tungsten filament which gives out intense white light.
For the UV region the source is a hydrogen discharge lamp.

→ A klystron or gun diode is used to generate microwave radiation.

→ The radiofrequency radiation is generated by causing an electric current to oscillate in a coil of wire.

<u>Modulator and Analyzer</u>:- The variation of absorption with frequency is determined by analyzing the spectral radiation by means of dispersing elements which separates different frequencies into rays that travel in different directions.

→ The simplest dispersing element is a glass or a quartz prism but a diffraction grating is most widely used.

→ A diffraction grating consists of glass or ceramic plate into which fine grooves have been cut out 1000 nm apart (a spacing comparable to the wavelength of white light) and covered with reflective aluminium coating.

→ The grating causes interference between waves reflected from its surface and constructive interferences occur at specific angles that depends upon frequency of radiation used.

→ Each wavelength of light is directed into a specific direction.

→ **Detector** :- A device that converts the spectral radiation (signal) into an electrical signal that passes to a recording device operating synchronously with the analyzer, thus producing either a trace on a chart recorder or a computer record of the spectrum.

→ common detectors are radiation-sensitive semiconductors.

→ The radiation is chopped by a shutter that rotates in the beam so that an alternating signal is obtained from the detector (an oscillating signal is easy to amplify than a steady signal).

→ A modulator is introduced to convert a signal of an AC and thus enhances the application of AC electronics to be employed in the recording stages.

→ In the microwave region the source is varied and analyzer is not needed much.

→ Low pressures and gaseous samples tends to show high resolution. The collisions between molecules is infrequent and hence reduced doppler broadening.

→ Microwave spectroscopy much relies on the gaseous samples.