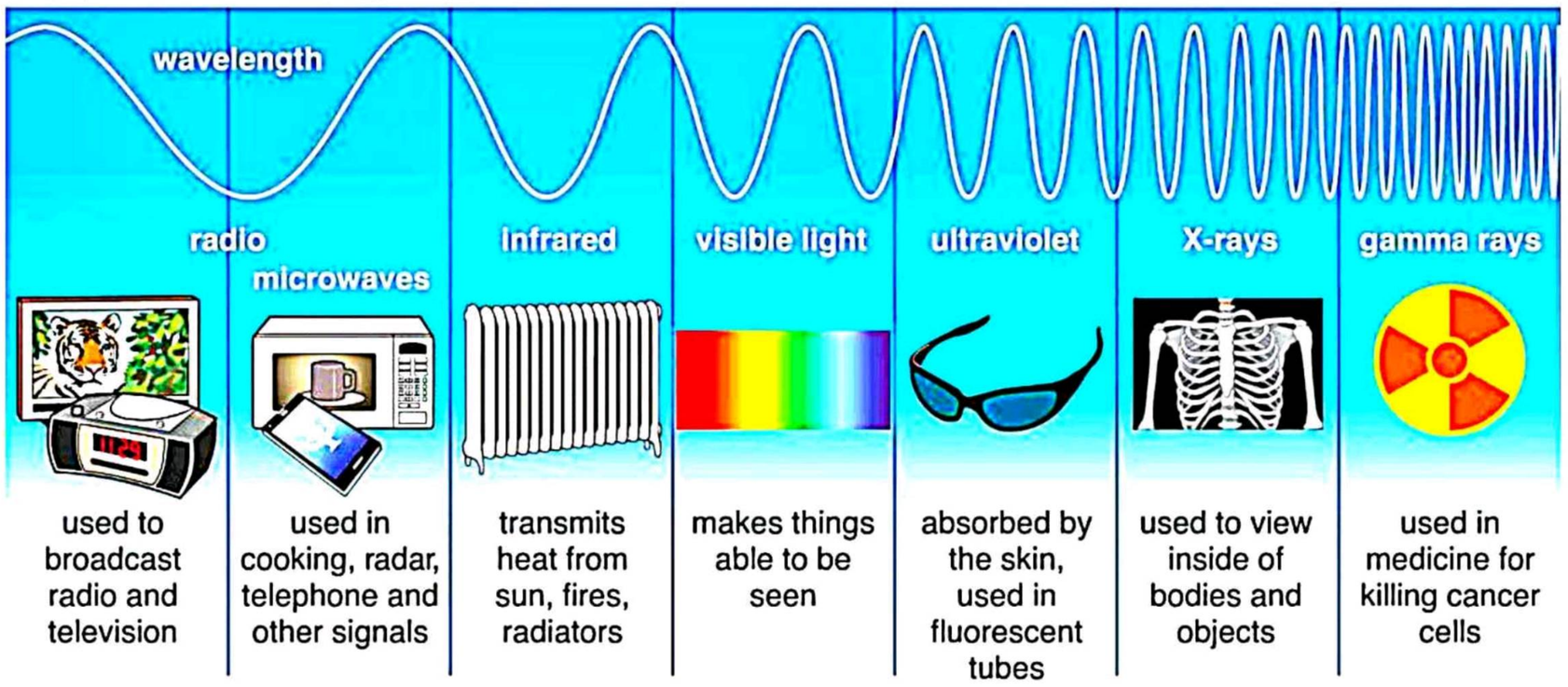
CHAPTER 13

SPECTROSCOPY



SPECTROSCOPY:

Spectroscopy is the study of interaction of electromagnetic radiation of light with matter. It's a powerful analytical technique for the determination of structure of molecules.

TYPES OF SPECTROSCOPY:

1. Infrared (IR) Spectroscopy
2. Ultraviolet/Visible (UV-Vis) Spectroscopy
3. Nuclear Magnetic Resonance (NMR) Spectroscopy
4. Atomic Absorption and Emission Spectroscopy
5. Mass Spectrometry

1. Infrared (IR) Spectroscopy

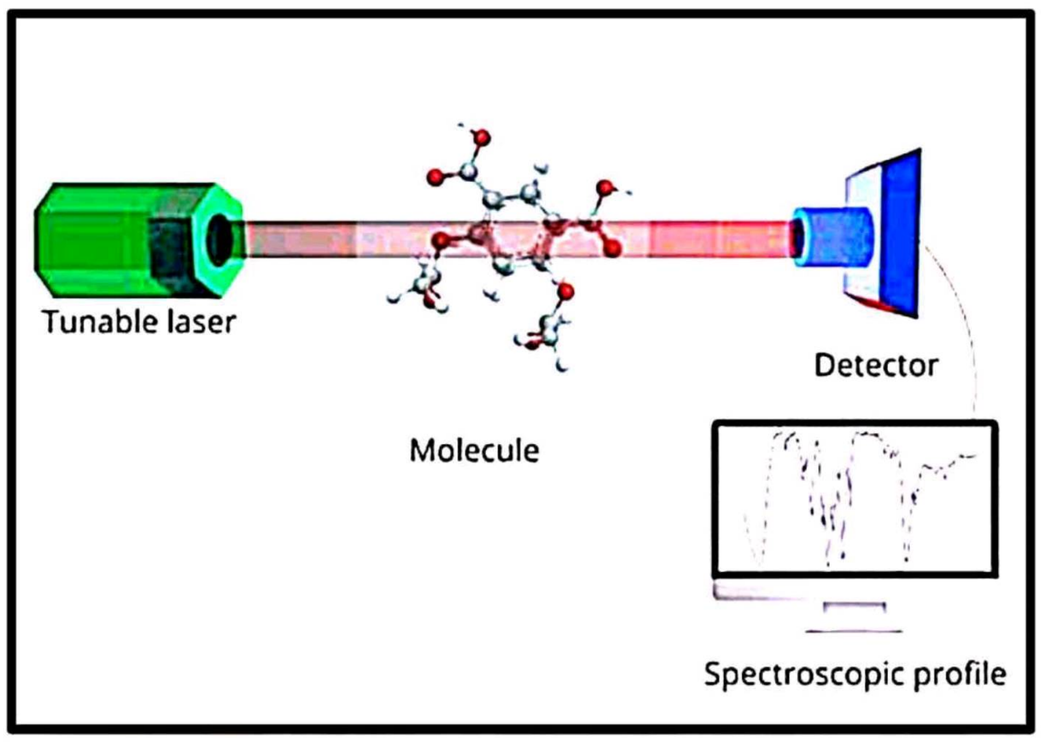
Infrared spectroscopy is used to detect the type of bond and the functional groups present in molecule. The atoms in a molecule already undergo vibration and rotation, in their normal routine, however when the molecules absorb radiations, it leads to increased intensity of vibrations. This vibration can be of two types namely **bond stretching** and **bond bending.** In bond stretching, the bond length increases or decreases while in bond bending the bond angle between the atoms changes.

The bending and stretching of each type of bond present in the molecule occurs at a particular frequency of IR spectrum and show the signals at a particular region.

The applications of IR spectroscopy are as follows:

(i) IR spectroscopy provides information for the presence of different functional groups in the organic molecules.

(ii) IR spectroscopy is also useful for identifying the impurities present in the sample to be analyzed.

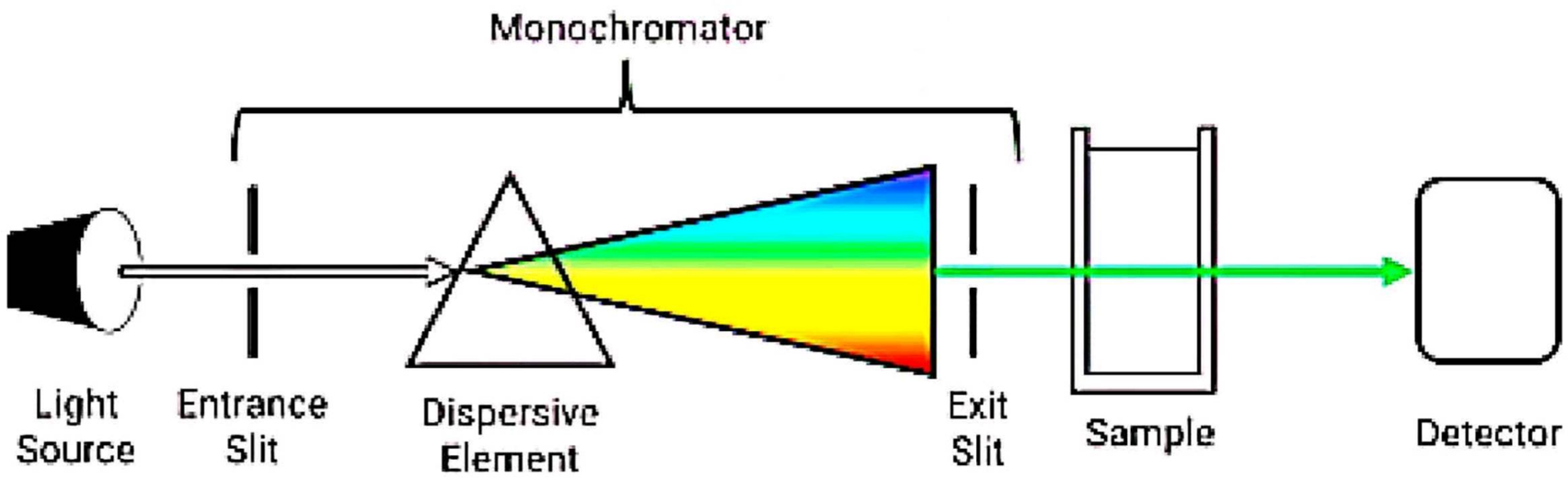


2. Ultraviolet/Visible (UV-Vis) Spectroscopy

It is used to determine the presence of double and triple bonds as well as conjugated system in the molecule. The UV region of electromagnetic spectrum extends from 200 nm to 400 nm and the visible region extends from 400 nm to 800 nm.

When a molecule absorbs electromagnetic radiations of UV – visible range (200 nm – 800 nm) electronic transitions occur. Its electrons are promoted from lower energy level to higher energy level.

UV spectroscopy is extensively used for determining the concentration of unknown compounds in a solution by using Beer-Lambert's law.



3. Nuclear Magnetic Resonance (NMR) Spectroscopy

The nucleus of certain elements exhibits random spin and behave like a tiny magnet due to their charged nature. When an external magnetic field is applied, the spin of nucleus aligned in two ways.

(i) It can align in the same direction of the applied magnetic field and it is said to be low energy spin state.

(ii) It can be opposite direction to the applied magnetic field and said to be high energy spin state.

When a sample of a compound is placed in a strong magnetic field and subjected to radio frequency radiation, the nuclei with specific spin state absorbs energy and flip into a high energy state, this absorption of energy is detected as signals in the NMR spectrum. The solvent used in NMR spectroscopy is usually D_2O or DMSO (Di Methyl SulfOxide)

The graph of NMR consists of the following parameters.

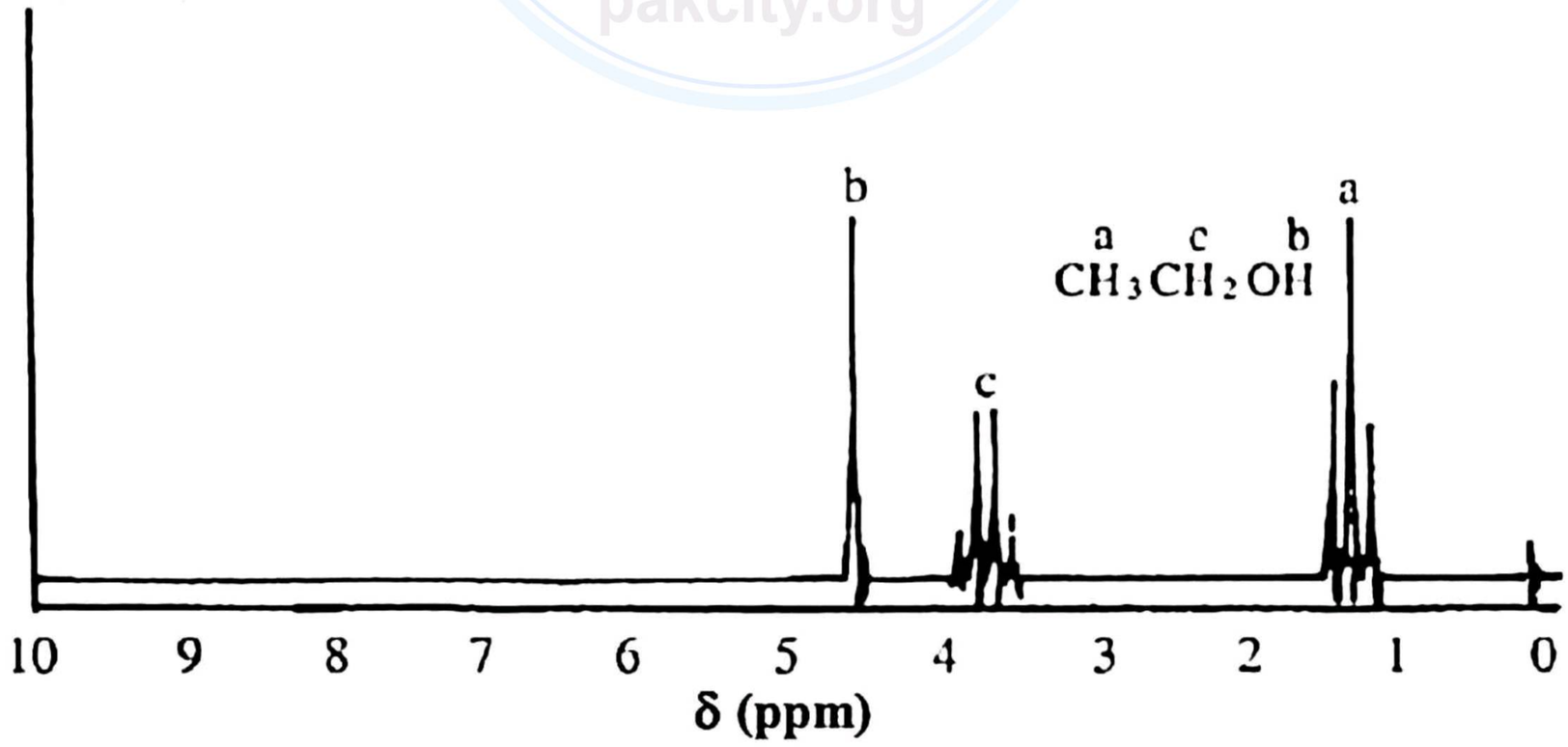
(i) x-axis represents chemical shift which shows position of proton signals relative to TMS (tetramethylsilane). The values are between 0 – 12 ppm relative to TMS.

(ii) y-axis represents absorption which shows the intensity of NMR signals.

(iii) Peak represents splitting pattern (singlet, doublet, triplet, quartet) due to neighboring protons.

Consider the example of ethanol

- Methyl (CH_3) protons appear as triplet around 1.1 to 1.3 ppm
- Methylene (CH_2) protons appear as quartet around 3.5 to 4 ppm
- Hydroxyl (OH) protons appears as a broad singlet around 4 to 5 ppm.



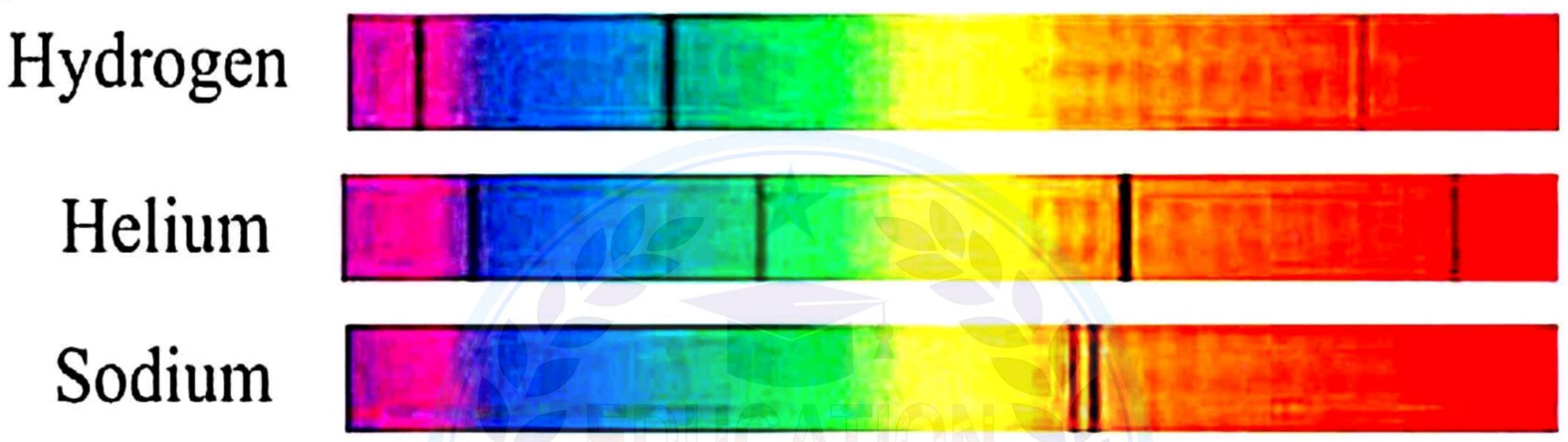
NMR spectroscopy provides valuable information about the chemical structure of organic compounds. Each organic compound exhibits a unique NMR spectrum acting as a 'fingerprint' that allows chemists to identify them.

4. Atomic Absorption and Emission Spectroscopy

It is used to identify elements in various samples including metal compounds. Within an atom, electrons are distributed in different energy levels, when atom receive energy from an external source like heat or an electric discharge, electrons can be promoted to higher energy level. These excited electrons then undergo transition involving the absorption or emission of electromagnetic radiations.

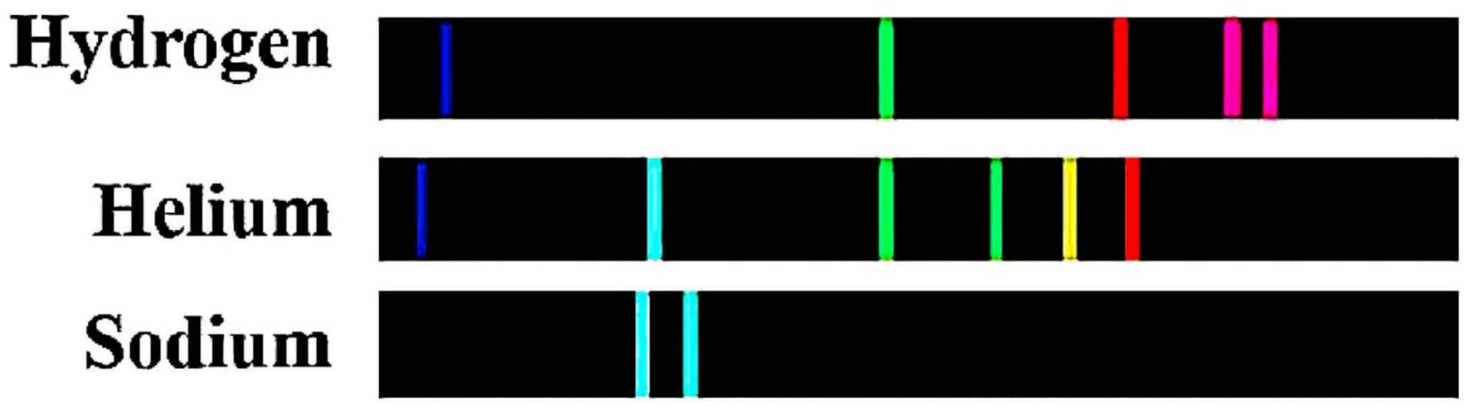
a) Atomic absorption spectroscopy

In atomic absorption spectroscopy, the sample is exposed to a wide range of light, the atom selectively absorbs specific wavelength of light that align with the energy needed to elevate electrons to higher energy level. The absorbed wavelength of light appears as dark lines in a unique pattern specific for that element. by examining the absorbed wavelength, a chemist can identify the presence of specific element in the sample.



b) Atomic emission spectroscopy

In atomic emission spectroscopy, the electron in an atom is first excited by providing energy from external source such as heat or electrical energy. When the excited electrons return to their ground state, they emit excess energy in the form of light of specific wavelengths. This emitted light appears as a series of bright lines against a dark background. Since each element has its distinct set of bright lines, chemist can identify the element based on this information.



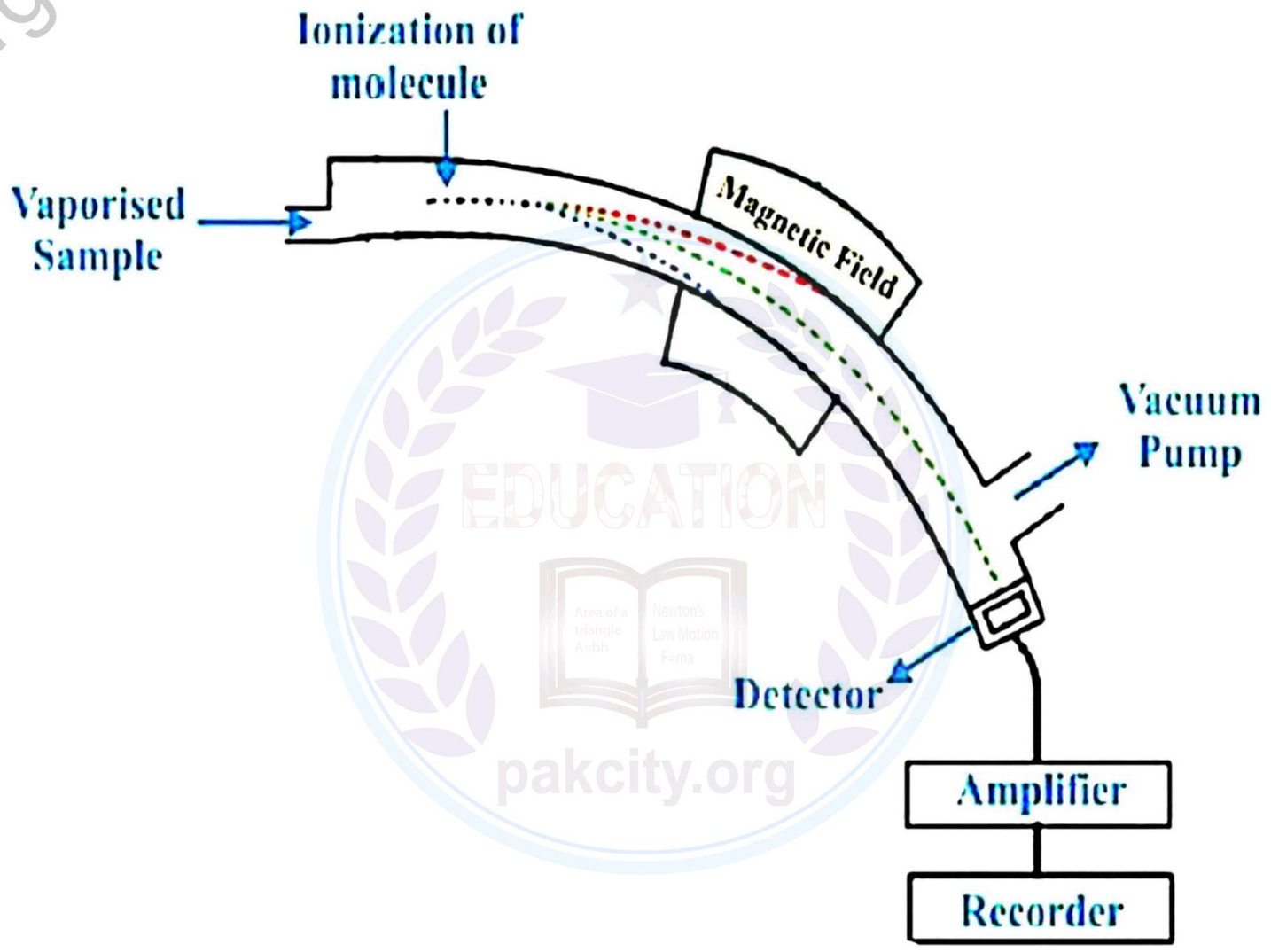
5. Mass Spectrometry

It is a technique used to determine the mass to charge ratio (m/z) of ions in a sample. It provides information about the mass of different fragments of the molecule.

In mass spectrometry, the vapors of compounds are bombarded with beam of high energy electrons from electron gun that makes the neutral molecules loose and electron and change into molecular ion. These molecular ion further break into smaller possible fragments of specific mass to charge ratio (m/z).

$$\underset{\text{(Neutral molecule)}}{Z} \xrightarrow{\text{high energy electron beam}} \underset{\text{(Molecular ion)}}{Z^{+}} + \bar{e}$$

These molecular ions then pass though magnetic field where they follow a curved path. A highly sensitive detector is attached in mass spectrometer which detects the molecular mass of ions and record on paper as specific lines.



It is used to determine the molecular mass of unknown compounds on the basis of mass to charge ratio.