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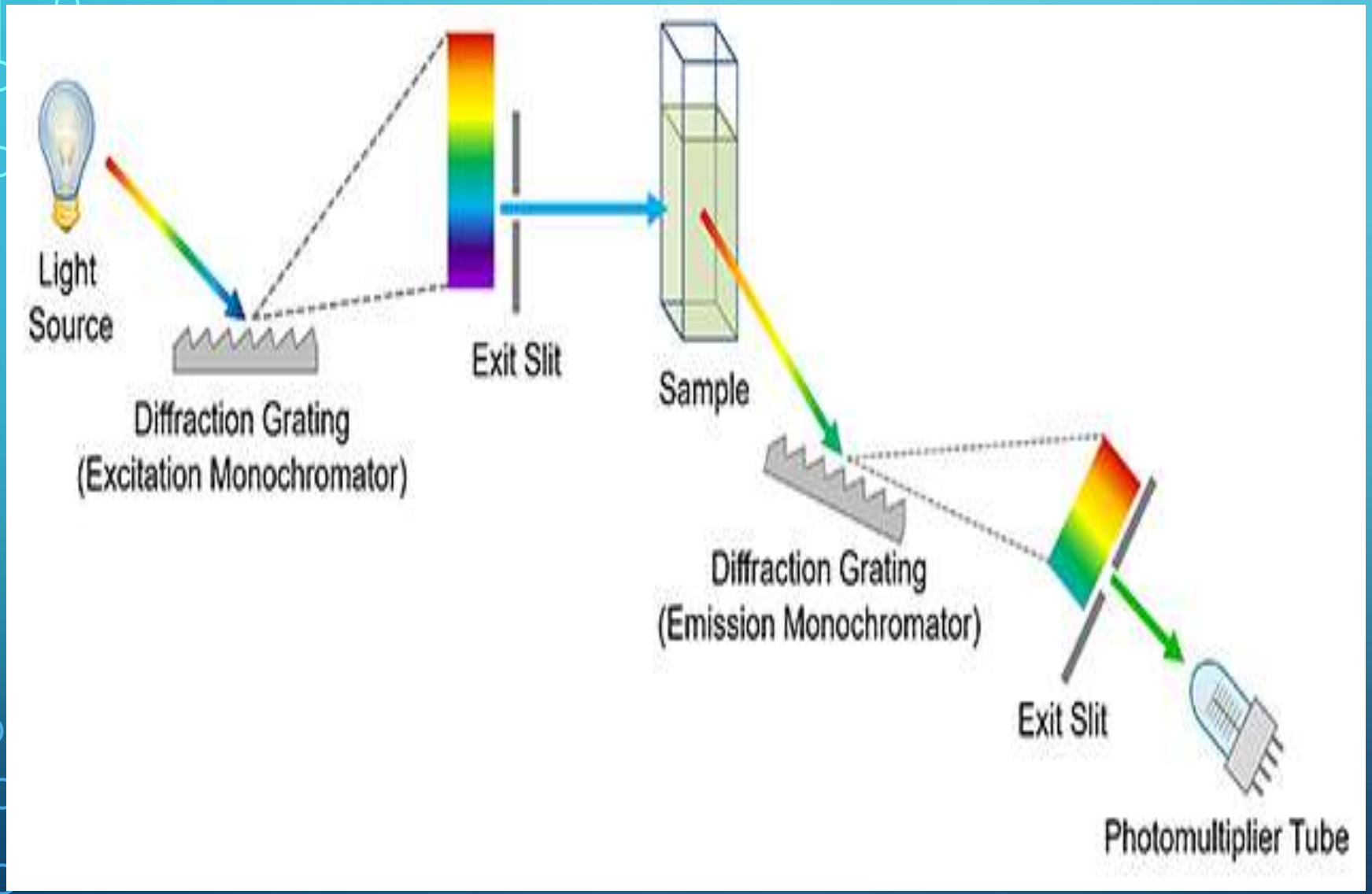

Light
Source
Diffraction Grating
(Excitation Monochromator)
Exit Slit
Sample
Diffraction Grating
(Emission Monochromator)
Exit Slit
Photomultiplier Tube

SPECTROSCOPY

CONTENT

- *Beer- Lambert law*
- *Light absorption and Transmission*
- *Extinction coefficient*
- *Application of UV-visible spectroscopic techniques*
- *Flame photometry*
- *Atomic absorption spectrophotometey*
- *Circular Dichroism*

- *Optical rotatory dispersion*
- *Principle and application of NMR and ESR techniques*

BEER-LAW

- *When monochromatic light passes through an absorbing medium its intensity decreases exponentially as the concentration of the absorption medium increases.*

$$I = I^{\circ} e^{-K2 C}$$

LAMBERT LAW

- *When a ray of monochromatic light passes through the absorbing medium its intensity decreases exponentially as the length of the absorbing medium increases.*

$$I = I^{\circ}\, e^{-k1\, l}$$

LIMITATION OF BEER-LAMBERT LAW

- *Only applicable to monochromatic radiations.*
- *Non-linearity arises at high concentration.*

LIGHT ABSORPTION

- *Definition*

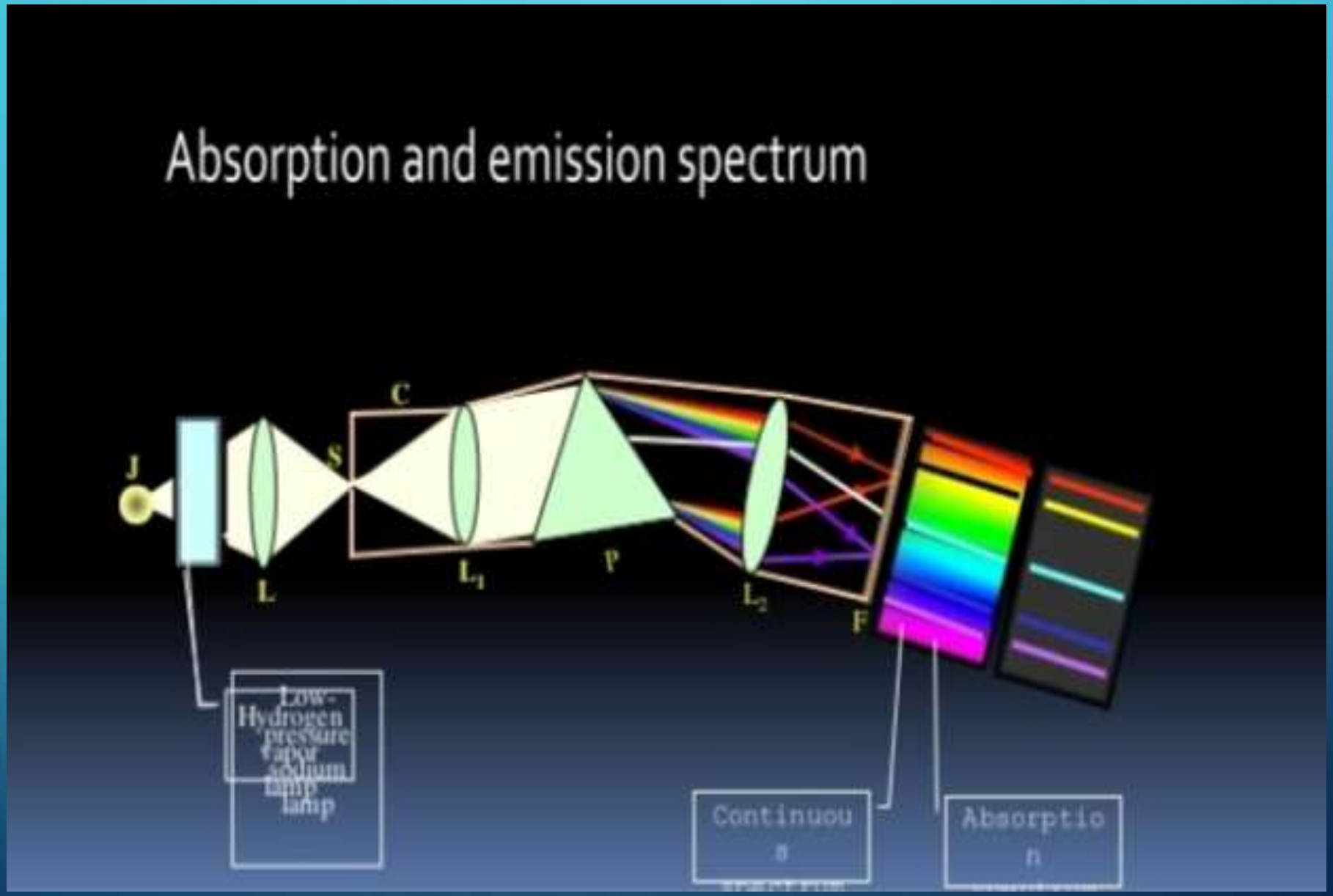
The phenomenon in which a medium decreases the intensity of the light beam going through it is called light absorption.

- *The law of light absorption*

The intensity of a monochromatic light beam after going through an absorbing medium decreases as an exponential function of the distance.

- *The selective absorption of light*

Different light are absorbed differently. In other words, the absorption of light through a medium is selective.


Absorption and emission spectrum
J
S
C
L
L_1
P
L_2
F
Low-
Hydrogen
pressure
vapour
sodium
lamp
Continuou
s
Absorptio
n

TRANSMISSION

Transmission of light is when light passes through an object depend on whether it is

- *Transparent*
- *Opaque*
- *Translucent*

TRANSPARENT

- *The transparent material allow light to pass through with almost no distance.*
- *It may or may not colour the light but clearly see objects through them*

Eg: Glass

TRANSLUCENT

- *Translucent material allow only part of the light to pass through, while also bouncing it in many new directions.*
- *It gives you a blurry view but lets in light.*

Eg: A frosted glass door (like a shower door)

OPAQUE

- *Opaque material completely block light from passing.*

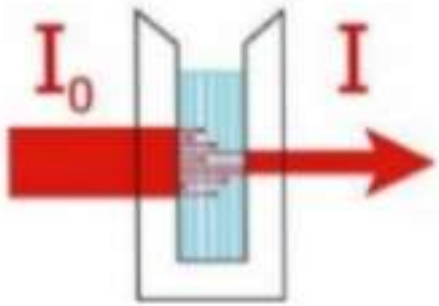
  Eg: Dark coloured cardstock paper

IMPORTANCE OF MOLAR EXTINCTION COEFFICIENT

- *Molar extinction coefficient is a measurement of how strong a chemical species absorb light at a given wavelength.*
- *The SI unit are m2 / mol but in practice they are usually taken as M -1 C -1*
- *Extinction coefficient allow us for estimation of molar concentration of solution from its measured absorbance.*

HOW TO FIND MOLAR EXTINCTION COEFFICIENT

- *Beer Lambert law use to find the molar extinction coefficient.*
- *The simple way to calculate it using the given formula.*



$$A = \log_{10} \frac{I_o}{I} = \varepsilon l c$$

$$\varepsilon = A/cl$$

concentration of solution (mol dm^{-3})

length of solution the light passes through (cm)

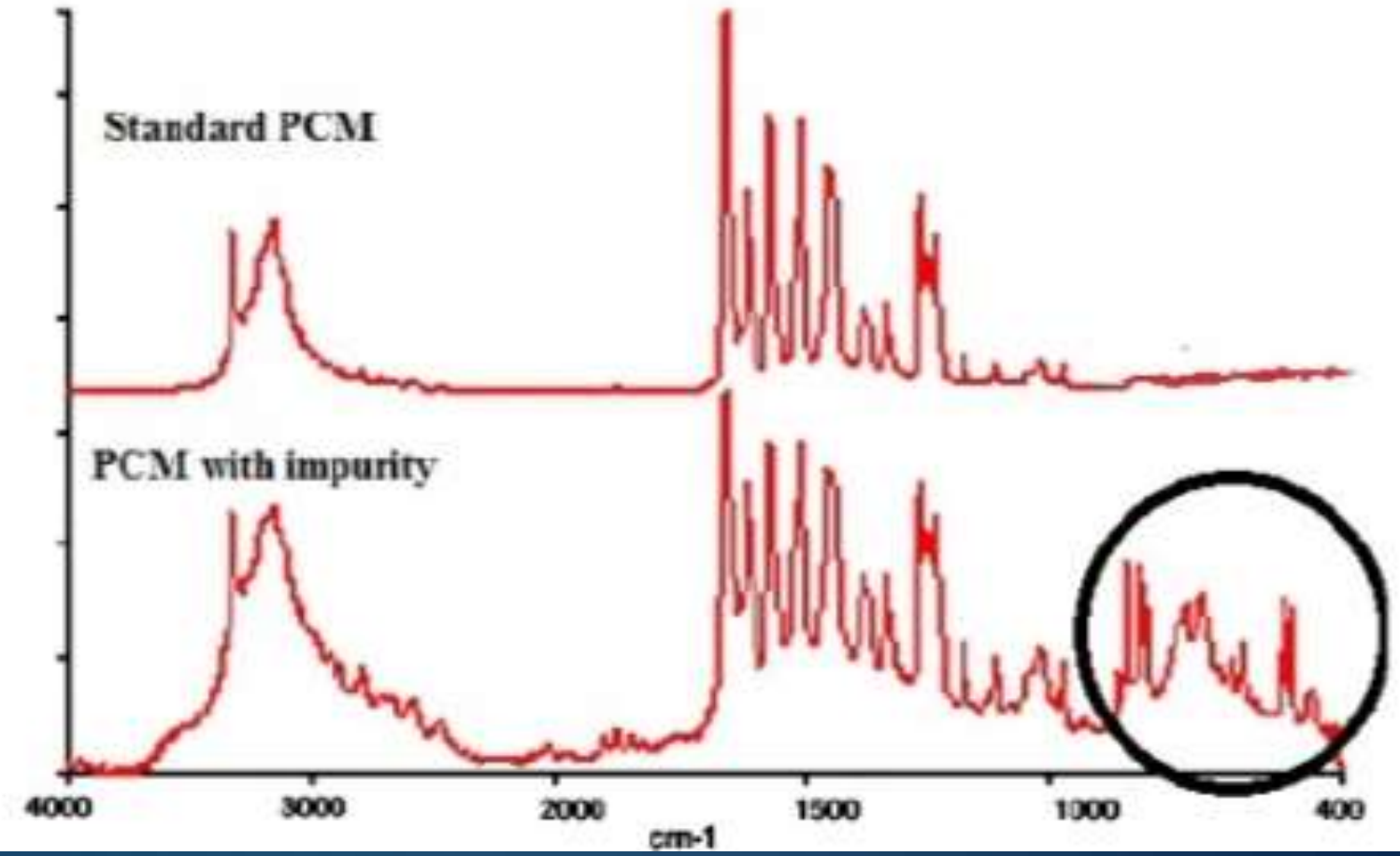
Where, I_0 is incident light, I is transmit light, ε is molar extinction coefficient, A represent absorbance, c is concentration, l is path length of light travel in the cuvette.

APPLICATION OF UV-VISIBLE SPECTROSCOPY

- *Detection of impurities.*

Uv absorption spectroscopy is one of the best methods for determining of impurities in organic methods. By also measuring the absorbance at specific wavelength, the impurities can be detected.

U.V. SPECTRA OF PARACETAMOL (PCM)

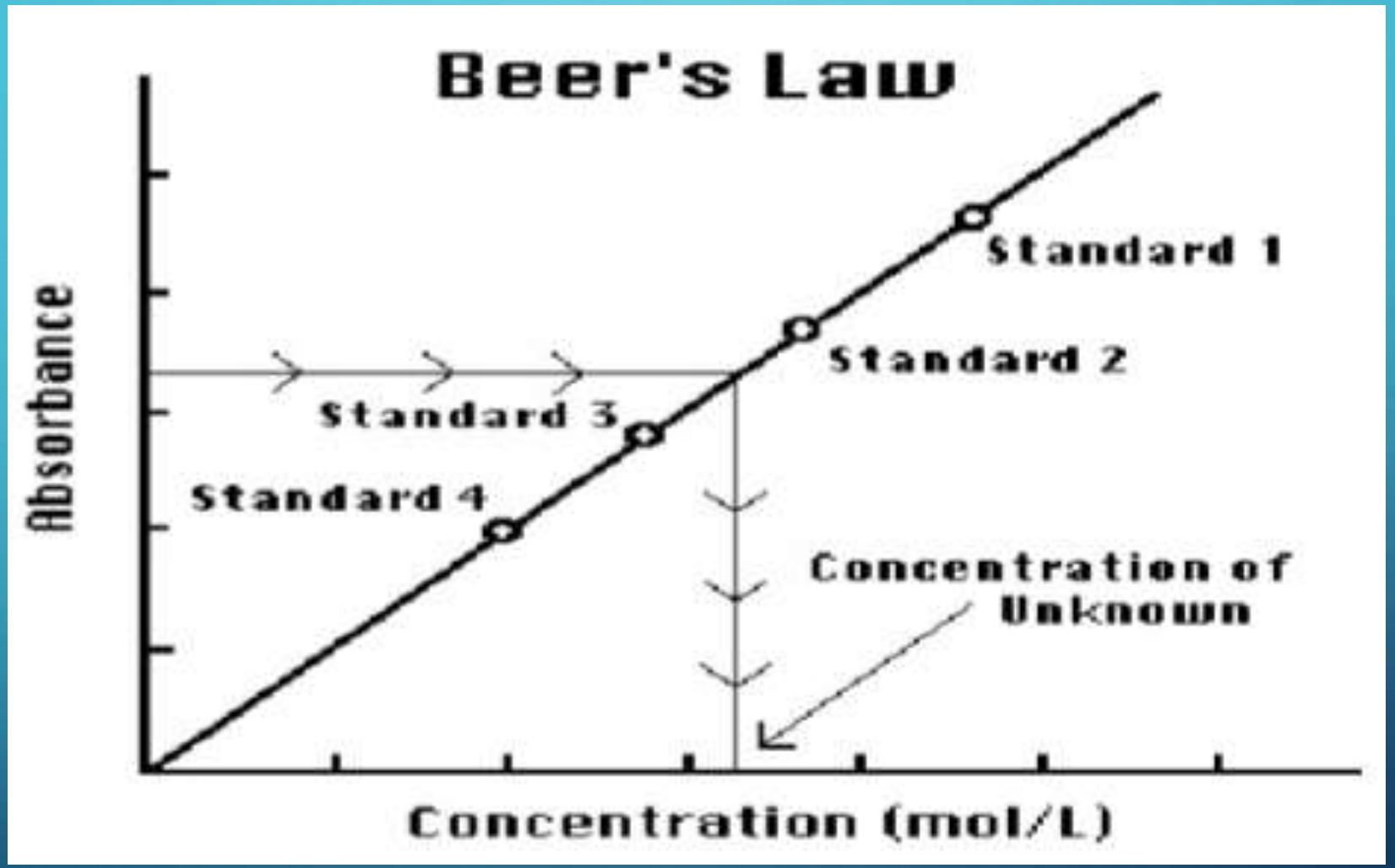


- *Structure elucidation of organic compounds.*

– *Uv spectroscopy is useful in the structure elucidation of organic molecules, the presence or absence of unsaturation,the presence of hetro atoms.*

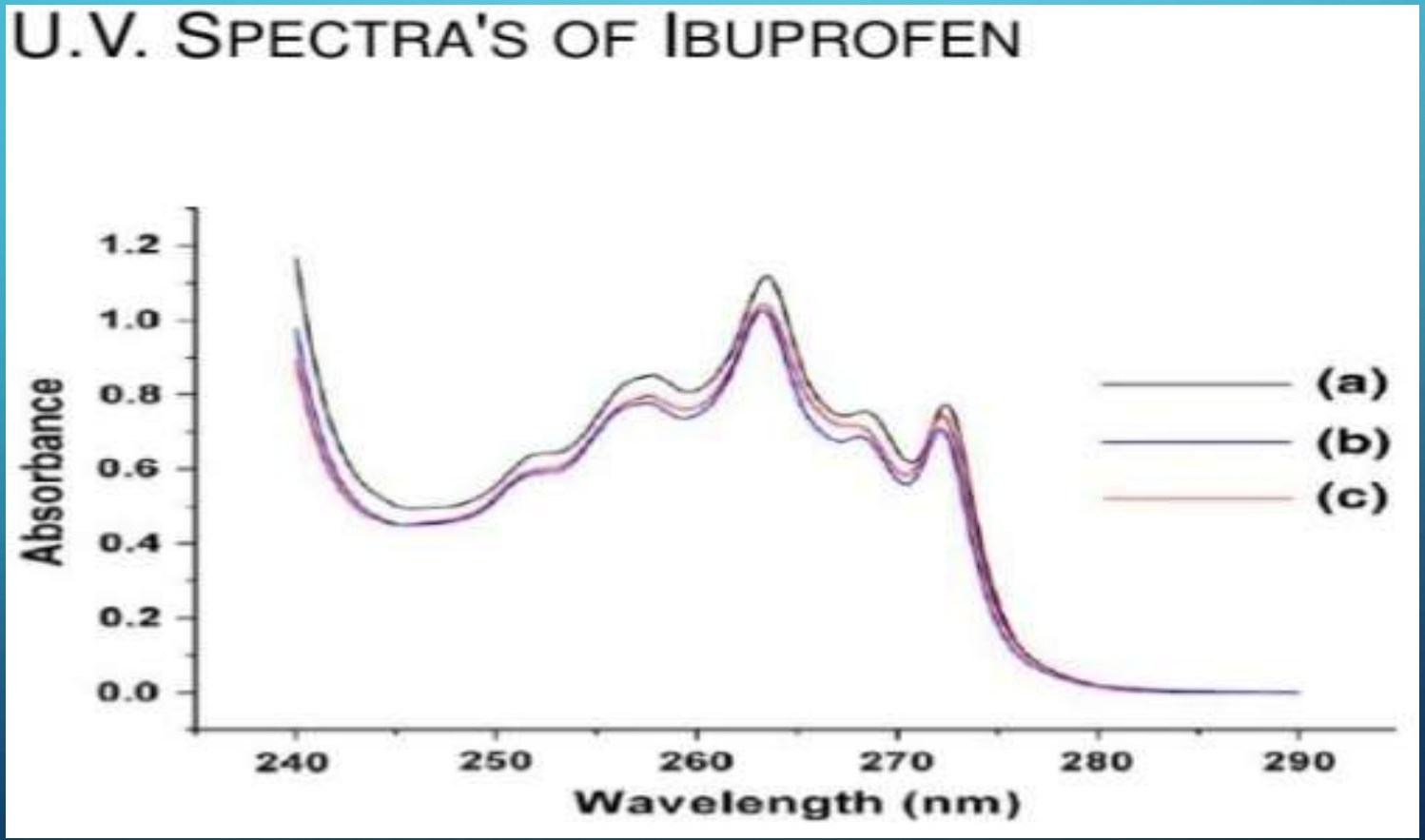
- *Quantitative analysis*

Uv absorption spectroscopy can be used for the quantitative determination of compounds that absorb uv radiation. This determination is based on Beer's law which as follows.


Beer's Law
Absorbance
Standard 1
Standard 2
Standard 3
Standard 4
Concentration of Unknown
Concentration (mol/L)

- *Qualitative analysis.*

Uv absorption spectroscopy can characterize those types of compounds which absorb uv radiation.



- *Chemical kinetics*

kinetics of reaction can also be studied using uv spectroscopy. The uv radiation is passed through the reaction cell and the absorbance changes can be observed.

- *Detection of fundamental group.*

To detect the presence or absence of function group in the compound

Absence of a band at particular wavelength regarded as an evidence for the absence of particular group.

- *Quantitative analysis of pharmaceutical substances.*

Many drugs are either in the form of raw material or in the form of formulation. They can be assayed by the drugs in a solvent.

- *Examinationof polynuclear hydrocarbons.*

Benzene and polynuclear hydrocarbons have characteristic spectra in ultraviolet and visible region.Thus identification of polynuclear hydrocarbons can be made by comparison with the spectra of polynuclear compounds.

- *As HPLC detector.*

A Uv /vis spectrophotometer may be used as a detector for HPLC.

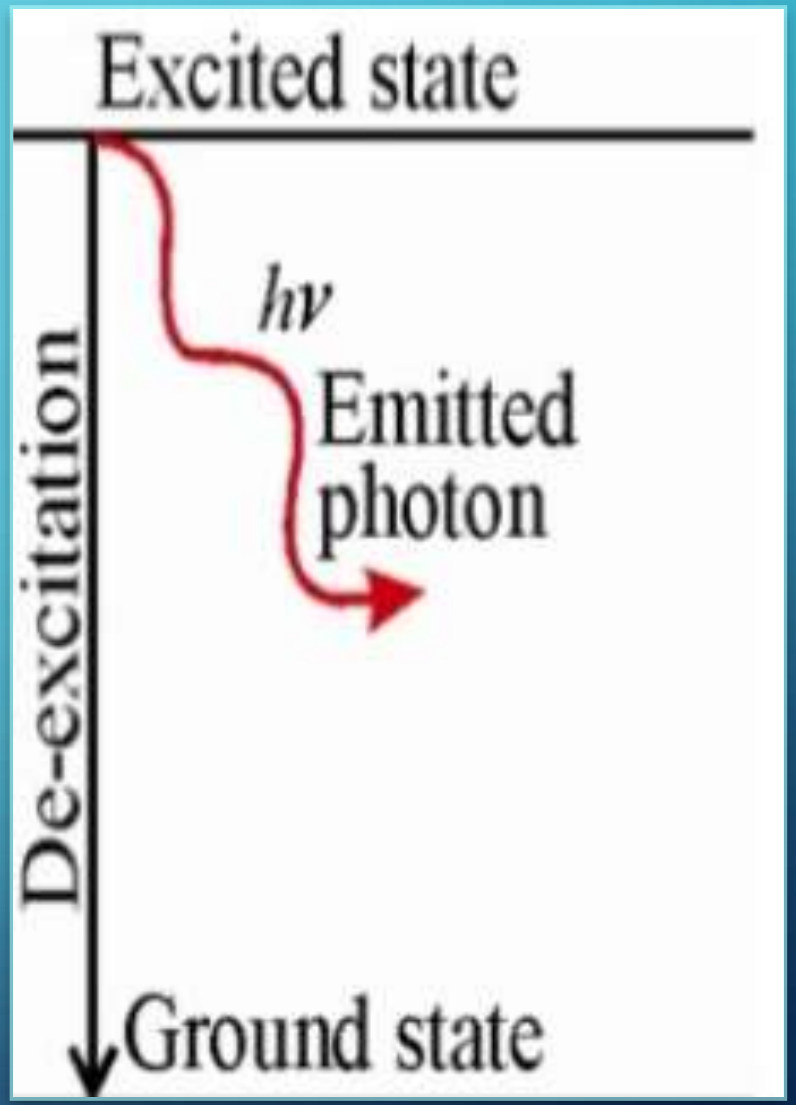
FLAME PHOTOMETRY

- *Flame photometry is also called Flame Atomic Emission Spectrometry is a branch of spectroscopy in which the species examined in the spectrometer.*

THE FLAME PHOTOMETER

BASIC CONCEPTS

- *Liquid sample containing metal salt solution is introduced into a flame.*
- *Solvent is first vaporized, leaving particles of solid salt which is then vaporized into gaseous state.*
- *Gaseous molecule dissociate to give neutral atoms.*



APPLICATION

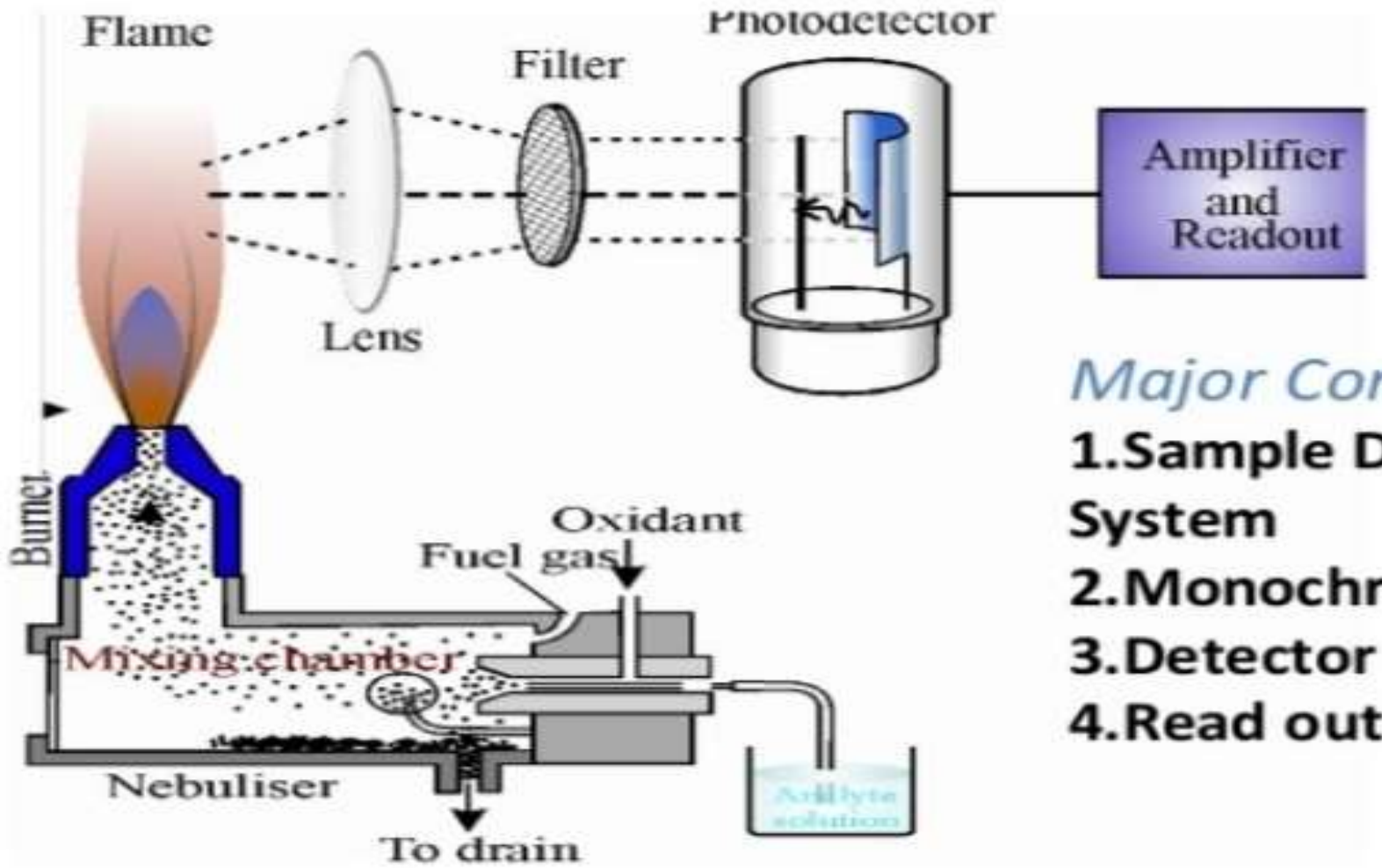
- *Flame photometry has both quantitative and qualitative applications.*
- *To estimate sodium, potassium, calcium, lithium etc.*
- *Flame photometry with mono-chromators emit radiation of characteristic wavelength which help to detect the presence of a particular metal in a sample.*

PRINCIPLES

- *When a solution is aspirated into a low temperature flame, in an aerosol ,each droplet of water evaporates leaving a solid of the residue of evaporation.*
- *Various metals emit a characteristic colour of light when heated.*

ELEMENT	EMISSION WAVELENGTH(nm)	FLAME COLOUR
Sodium(Na)	589	yellow
Potassium(K)	766	violet
Barium(Ba)	554	Lime green
Calcium(Ca)	662	orange
Lithium(Li)	670	Red

Schematic Representation of the Flame Photometer



Major Components:

1. Sample Delivery System
2. Monochromator
3. Detector
4. Read out device

ATOMIC ABSORPTION SPECTROSCOPY

- *Atomic absorption spectroscopy is a very common technique for detecting metals and metallic in samples.*

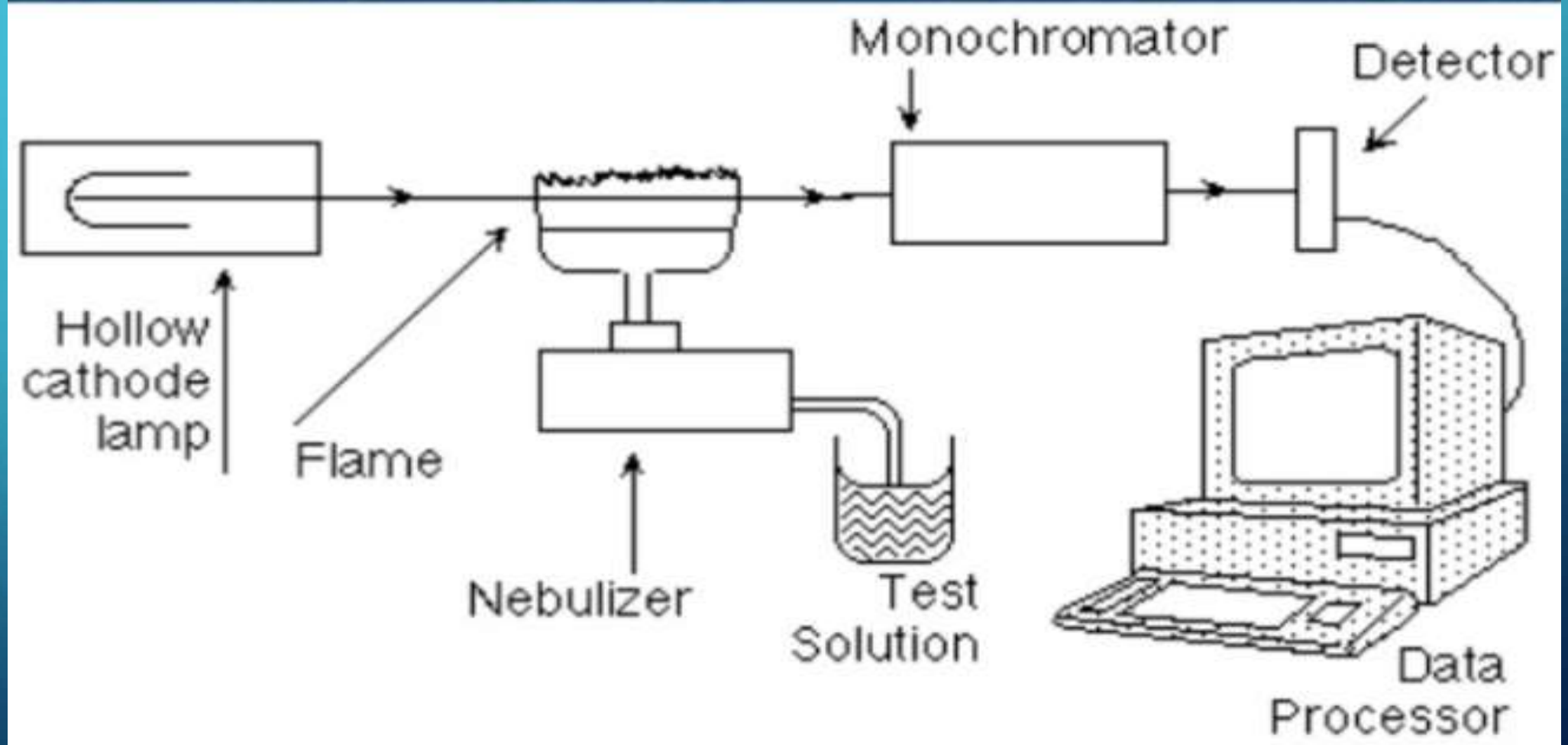
HISTORY

- *First atomic absorption spectroscopy was built by CSIRO scientist,Alan walsh in 1954, shown in the picture below.*

PRINCIPLES

- *The technique used basically the principles that free atoms(gas)generated in an atomizer can absorb radiation at specific frequency.*
- *Atomic absorption spectroscopy qualifies the absorption of ground state atoms in the gaseous state.*
- *The atoms absorb ul4or visible light and make transitions to higher electronic energy levels.*

Schematic diagram of AAS:

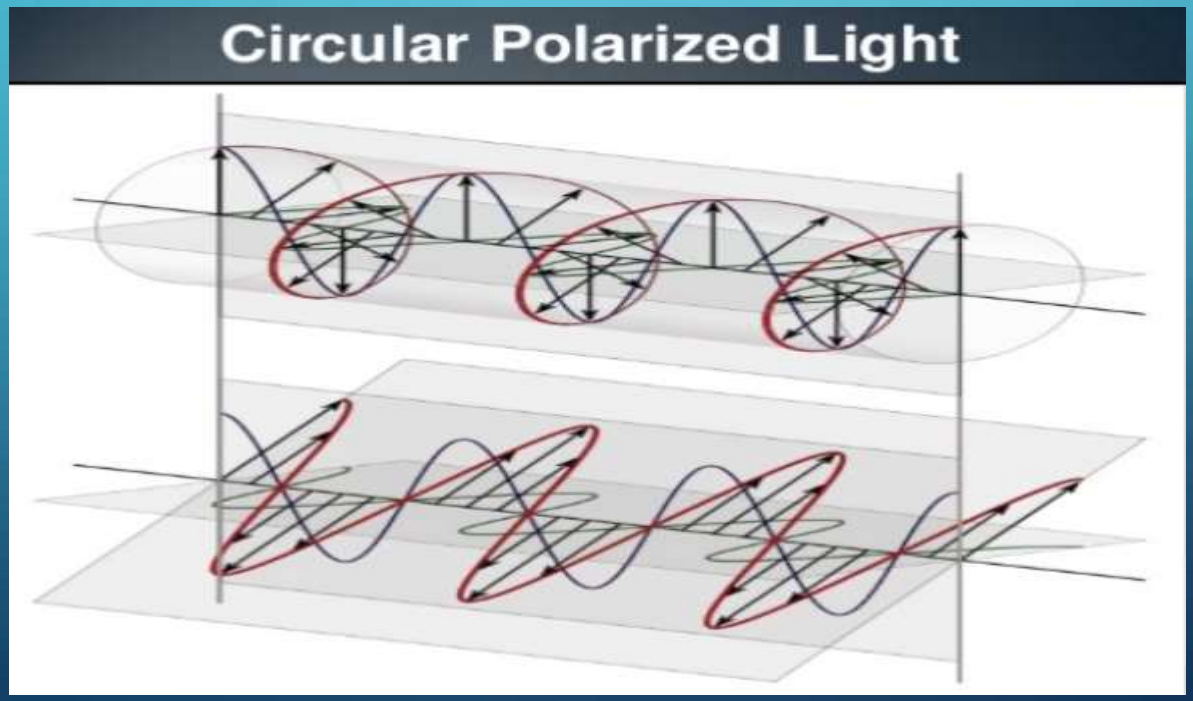


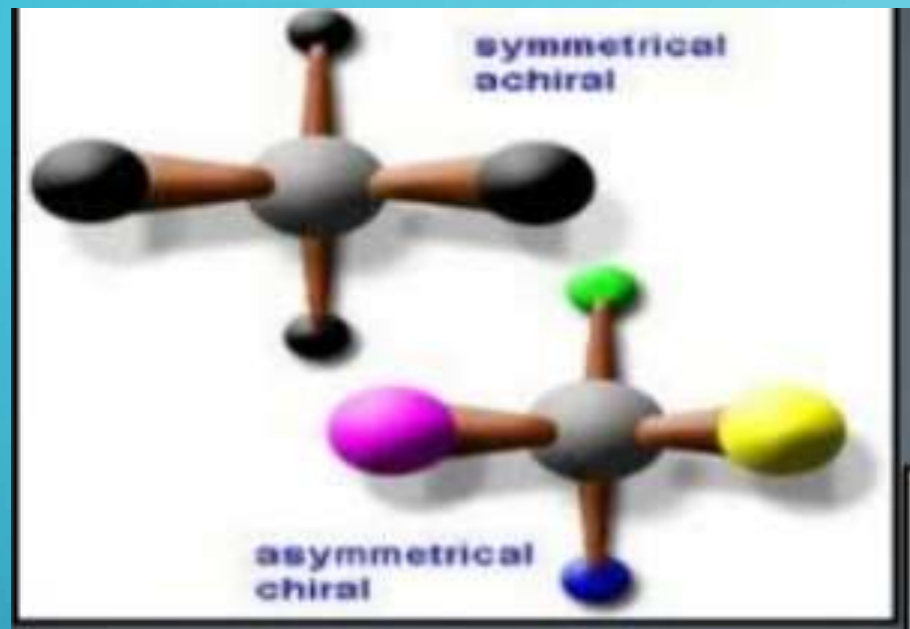
APPLICATION

- *Determination of even small amounts of metals(lead,mercury, calcium, magnesium etc.)*
- *Environmental studies:drinking water,ocean water, soil.*
- *Food industry*
- *Pharmaceutical industry.*

CIRCULAR DICHROISM

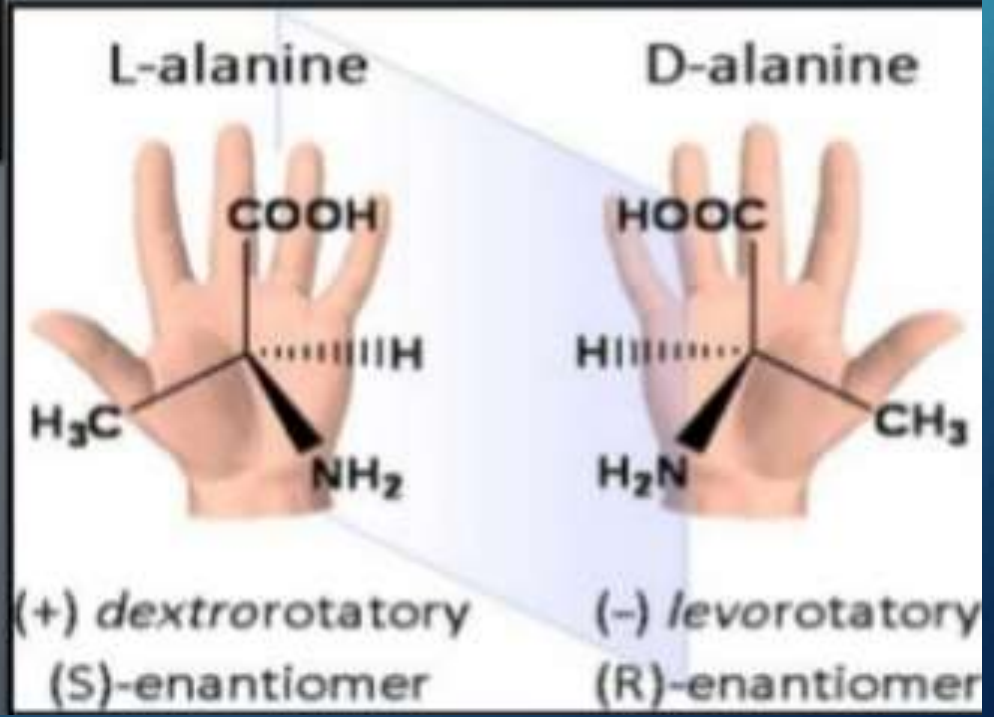
- *Circular Dichroism spectroscopy is a form of light absorption spectroscopy that measures the difference in absorbance of right-left circularly polarized light.*



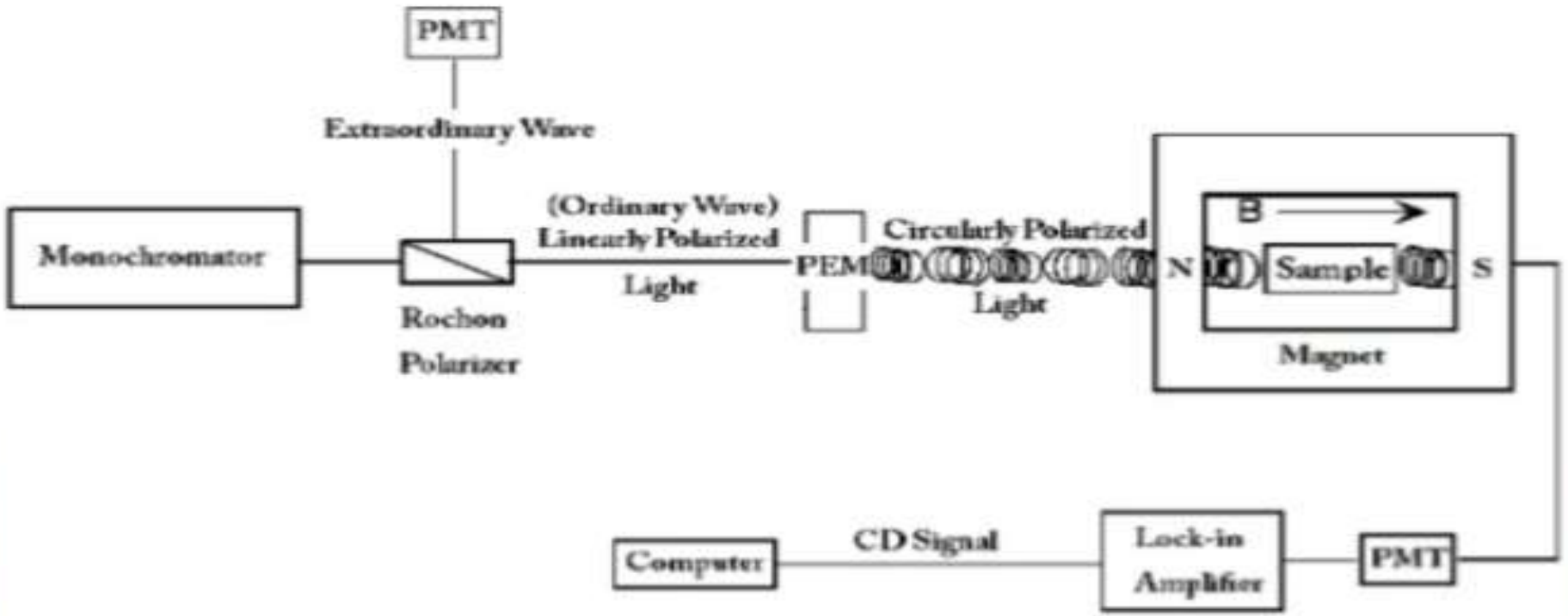


Asymmetry

Optical activity



Block diagram of CD spectropolarimeter.



APPLICATION

- *Circular Dichroism phenomena that result when a symmetrical molecules interact with plane polarized light.*

OPTICAL ROTATORY DISPERSION

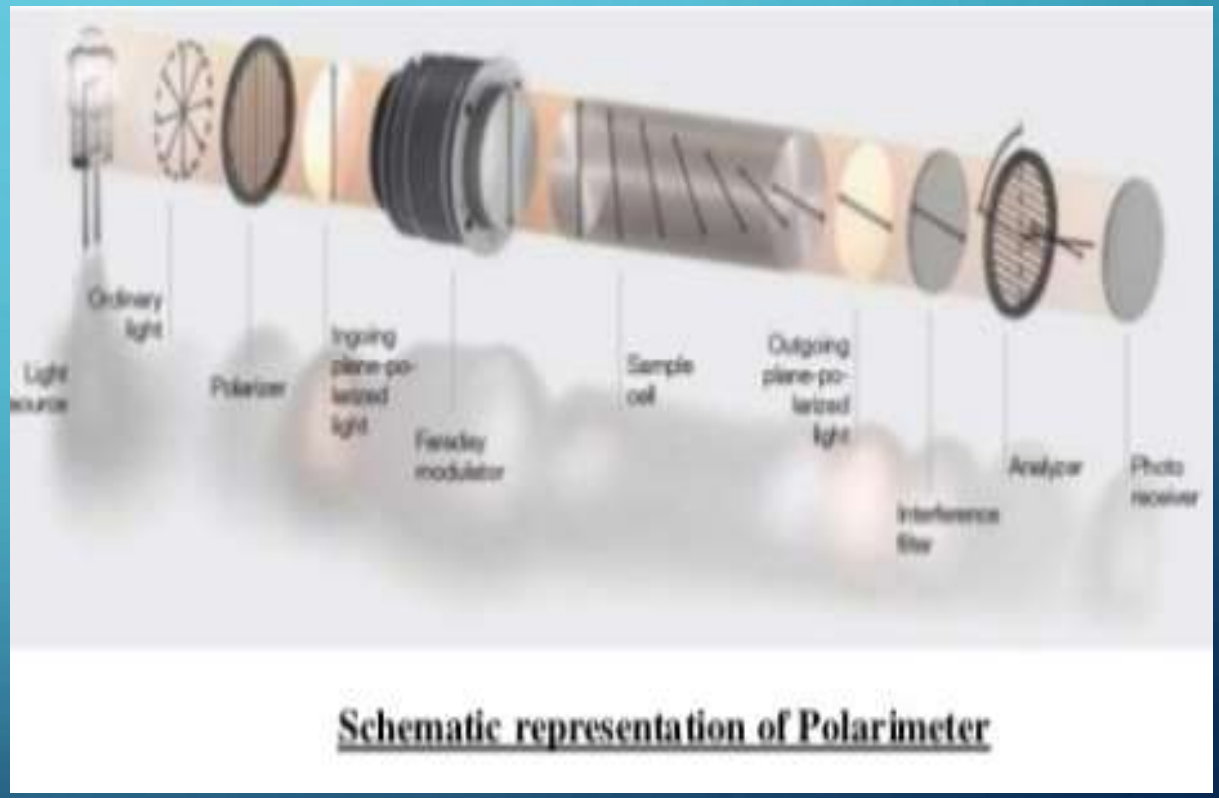
- *Optical rotatory dispersion is the variation in the optical rotation of a substance with a change in the wavelength of light.*

FUNDAMENTAL OF ORD

- *Plane / linearly polarized light.*
- *Optical activity.*
- *Specific rotation.*
- *Circular Birefringence / optical rotation.*

INSTRUMENTATION OF ORD

- *Light source*
- *Monochromater*
- *Polarizer*
- *Analyzer*
- *Sample tube*
- *Photo multiplier*



Schematic representation of Polarimeter

APPLICATION

- *Quantitative analysis: Specific rotation is a good measure of concentration.*
- *Determination of absolute configuration. Configuration studies. Eg: (+) 3 methyl cyclohexanone.*

PRINCIPLES OF ESR

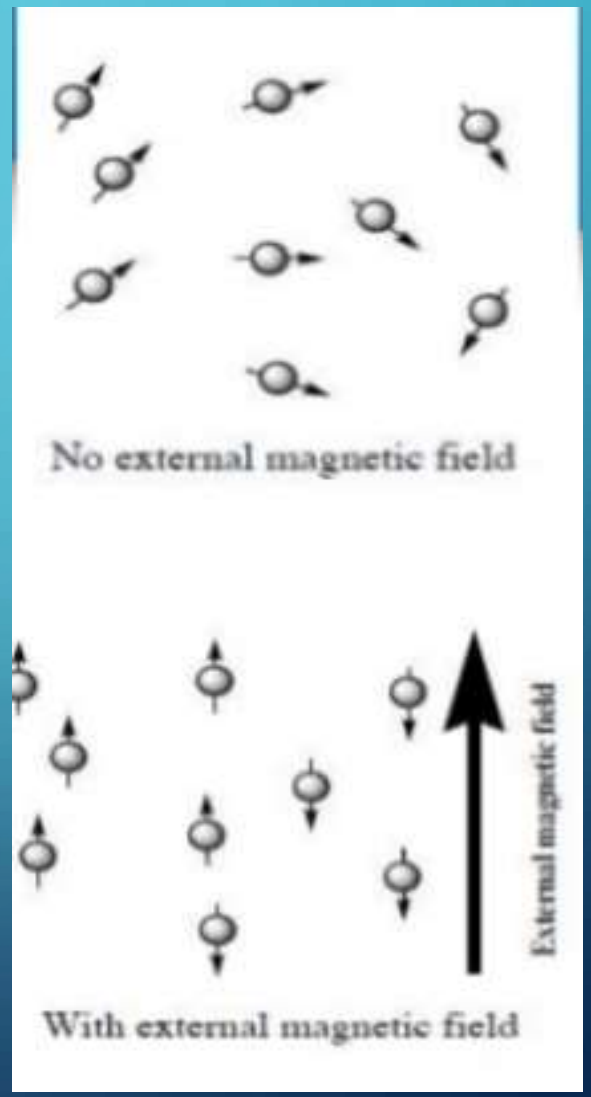
- *The study of the behaviour of the electrons in a given information about the condition of the sample.*
- *ESR is used to observe and measure the absorption of microwave energy by unpaired electrons in a magnetic field.*

APPLICATION OF ESR

- *ESR /EPR spectroscopy is used in various branches of science, such as biology, physics, chemistry, for the detection and identification of free radicals and para magnetic centres such as F-centers.*
- *EPR is a sensitive, specific method for studying both radicals formed in chemical reaction and the reaction themselves.*

PRINCIPLES OF NMR

- *The principles behind NMR is that many nuclei have spin and all nuclei are electrically charged. If an external transfer is Possible between the base energy to a higher energy level.*



APPLICATION OF NMR

- *Nuclear magnetic resonance spectroscopy is widely used to determine the structure of organic molecules in solution and study molecular physics, crystal as well as non-crystalline materials.*
- *NMR is also routinely used in advanced medical imaging techniques, such as in magnetic resonance imaging (MRI).*


thank you