INTRODUCTION TO SPECTROSCOPY AND APPLICATIONS IN NMR SPECTROSCOPY

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ABOUT

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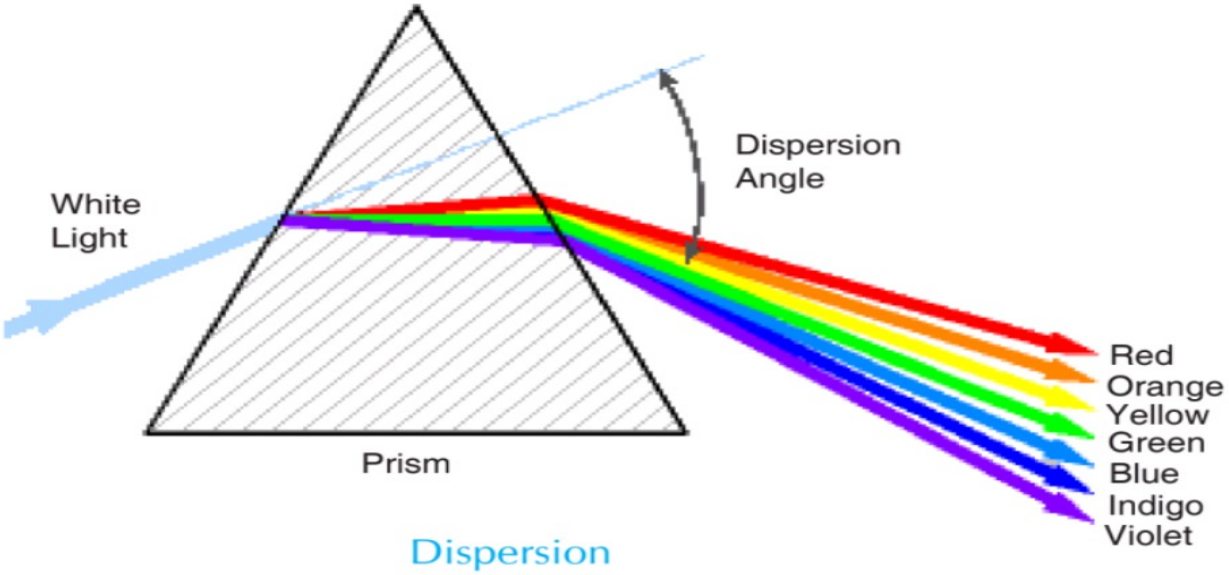


INTRODUCTION TO SPECTROSCOPY

DEFINITION & CLASSIFICATION

- The branch of science dealing with the study of spectra is called spectroscopy. "Spectro" means radiation and "Scopy" means measurement and Spectroscopy means Measurement of Radiation.
- The series of colour bands is called a spectrum. Ex : Light is a spectrum of radiation.
- The splitting of light into series of colour band is known as dispersion.

when visible light of a group of electromagnetic radiations is passed through a prism, it is split up into seven colours which correspond to definite wavelength. This phenomenon is called dispersion.



Dispersion

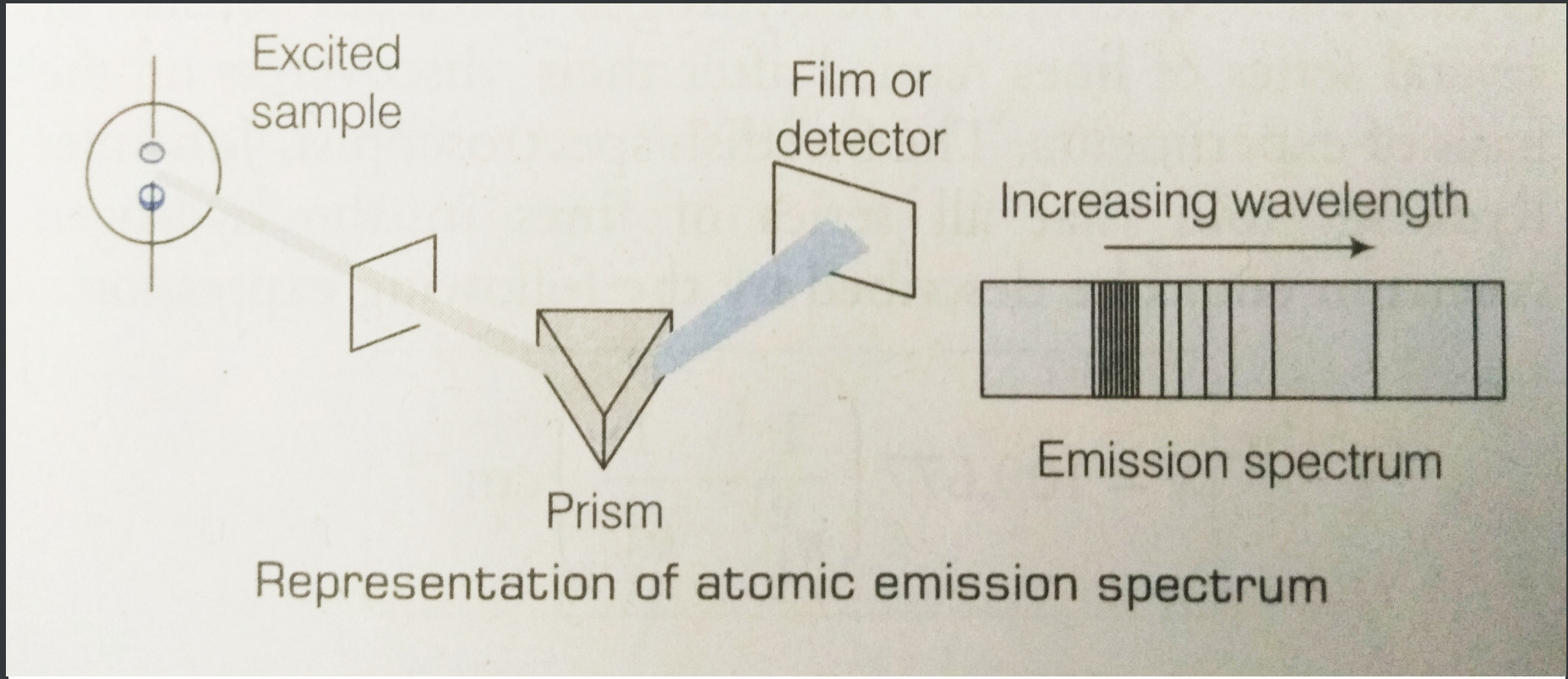
CLASSIFICATION OF SPECTROSCOPY

- **EMISSION SPECTROSCOPY**

The spectrum of radiation emitted by a substance that has absorbed energy either by passing electric discharge through a gas at low pressure (or) by heating the substance to high temperature is called an emission spectrum.

Atoms, molecules or ions that have absorbed radiation is called excited state.





Representation of atomic emission spectrum

EMISSION SPECTROSCOPY

CLASSIFICATION OF THE EMISSION SPECTRA

CONTINUOUS SPECTRUM : Such spectrum have continuity of colours, one colour merges with another colour without any gab or discontinuity. Ex : Light passed on the substance.

LINE OR ATOMIC SPECTRUM : The emission spectra of atoms in the gas phase emit light only at certain specific wavelength with dark spaces between them. Such spectra is called Line spectra or Atomic spectra. The emitted radiation is identified by the appearance of bright lines in the spectra. Ex : The emission spectra of Na consists of 2 yellow lines at 589.6 nm.





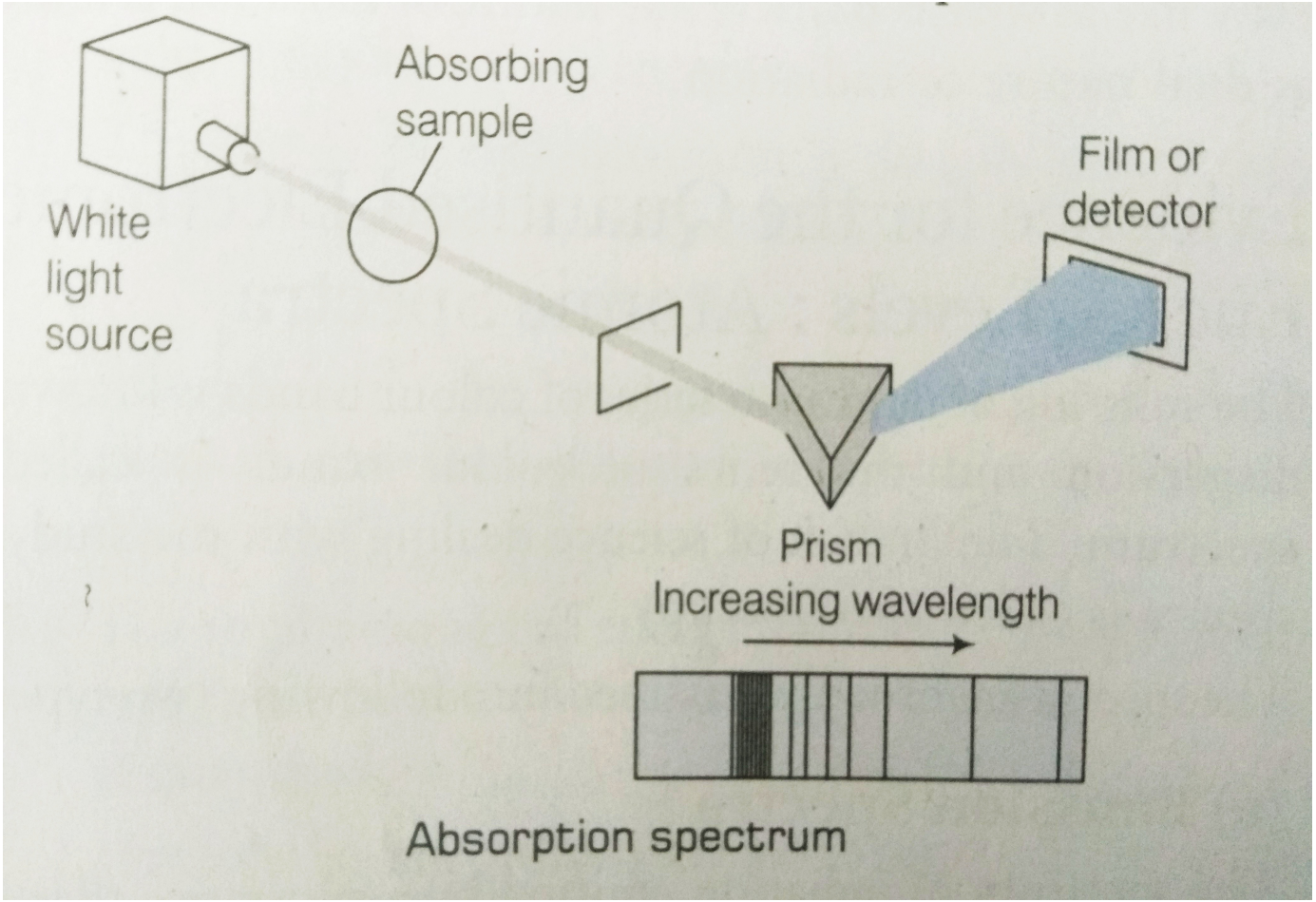
CLASSIFICATION OF SPECTROSCOPY

- **ABSORPTION SPECTROSCOPY**

It is the photographic negative of an emission spectrum. To obtain an absorption spectra a continuum of radiation is passed through a sample which absorbs radiation of certain wavelength.

To missing wavelength with corresponds to the radiation absorbed by matter, leave dark spaces in the bright continuous spectrum.




Absorbing
sample
White
light
source
Film or
detector
Prism
Increasing wavelength
Absorption spectrum

PRINCIPLE OF SPECTROSCOPY

① All organic compounds interact with electromagnetic radiation and absorbs energy.

② Molecule absorbs energy temporary or permanent.

③ Absorbs Low energy radiation - molecular rotation or bond vibration.

④ Absorbs High energy radiation - promotion of electrons to higher energy level or bond cleavage.

⑤ Trainformation involves molecular rotation, bond vibration, electronic transition.

⑥ Molecule absorbs only the wavelength of radiation exactly the energy necessary for the transition.



IMPORTANT CONCEPTS INVOLVED IN SPECTROSCOPY



a) ELECTROMAGNETIC RADIATION OR ELECTROMAGNETIC WAVES

b) WAVELENGTH

c) WAVENUMBER

d) FREQUENCY

e) ENERGY

What is wave ?

Definition : It is defined as the disturbance that originate from some vibrating source and travel outwards as a continuous sequence of alternating crest and trough.

What is wave motion ?

The wave originate from the centre of disturbance and propagate in the form of up and down movements. The point of maximum upward displacement is called crest. The point of maximum downward is called trough.

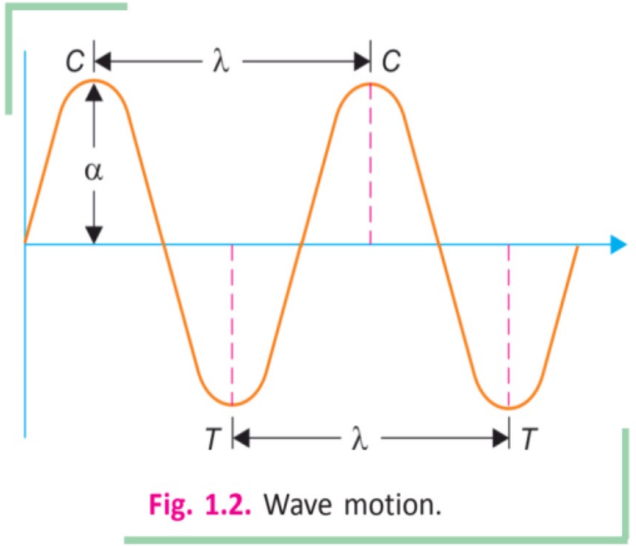


Fig. 1.2. Wave motion.

C - is the crest

T - is the trough

A - is the amplitude

Lambda - is the wave

WAVELENGTH (LAMBDA)

The distance between two adjacent crests (C-C) or troughs (T-T) in a particular wave is called wavelength. It has the unit of length. Since, different kinds of waves are of much smaller wavelengths so smaller units of length are used to describe them. It is generally expressed in terms of Angstrom (A°) or in Millimicrons (mu).

1 A° = 1 mu = 10 power -8 cm = 10 power -10 m

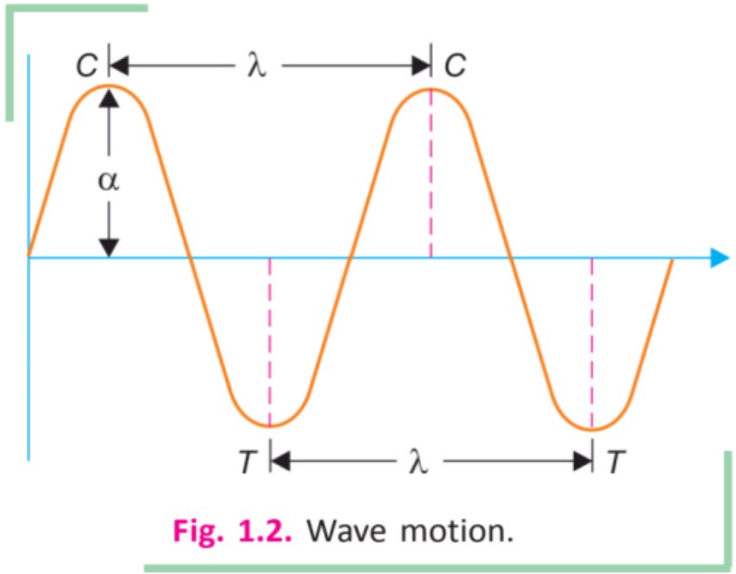
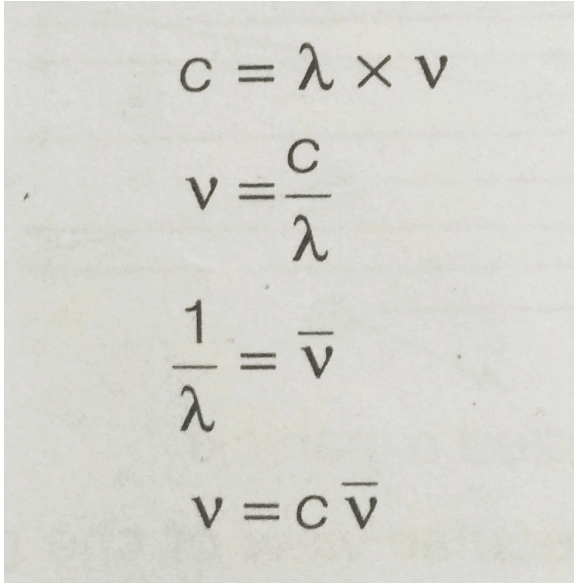


Fig. 1.2. Wave motion.

WAVENUMBER (V`)

It is defined as the number of wavelengths per unit length. Its unit is reciprocal of wavelength

Unit : m power -1 or commonly used unit is cm power -1 (it is not SI unit)





FREQUENCY (V)

It is defined as the number of waves that pass through a given point in one second. It unites are cycles per second or simply reciprocal of seconds. SI unit : Hertz (Hz) after the name of Heinrich Hertz.

1 Hz = 1 cycle per second

V = C / Lambda

A cycle is said to be completed when a wave consisting of crest and trough pass through a point.

Greater the wavelength, Smaller the frequency.





VELOCITY (C)

It is the distance traveled by a wave in one second.

Unit : ms power -1

In vacuum all types of electromagnetic radiations of wavelength travel with the same speed (3.0 × 10 power 8 ms power -1). This is called speed of light (c).





ENERGY (E)

Energy of a wave of the particular radiation can be calculated by applying the relationship :

E = hv
E = h.c/Lambda

h - is the planck constant (h = 6.626 × 10 power -27 erg secs.
v - is the frequency of radiation cycles per second
c - is the velocity of electromagnetic radiation or light
Lambda - is the wavelength in cm



ENERGY OF LIGHT & RELATIONSHIP BETWEEN ENERGY OF PHOTON, QUANTUM AND EINSTEIN

E (ENERGY) = hv (PHOTON)

E = hv

[v = c / Lambda]

E = hc / Lambda

E = hc. 1/ Lambda [v` = 1 / Lambda]

E = hcv`

Frequency (v) :

v = c / Lambda

Velocity (c) :

c = v × Lambda

Wavelength (Lambda) :

Lambda = c / v

Wavenumber (v`) :

v` = 1 / Lambda







What is Electromagnetic Radiation ?

Electromagnetic radiations are produced by the oscillation of electric charge and magnetic field residing on the atom. Light is an example for electromagnetic radiation or electromagnetic spectrum. Visible light is a form of energy. It was explained by two theories

1.) Corpuscular Theory and 2.) Wave Theory

According to wave theory, (Wave nature of electromagnetic radiation) :

James Clark Maxwell in 1870 gave an explanation about "interaction between charged bodies and the behaviour of electrical and magnetic fields on macroscopic level".

When electrically charged particles moves under acceleration, it will alternating electrical and magnetic fields are generated and transmuted in the forms of waves called the electromagnetic waves or electromagnetic radiation.

LET'S SEE CLASSIFICATION OF SPECTROSCOPY IN THE NEXT PRESENTATION

THANK YOU ALL



