TECHNIQUES IN BIOCHEMISTRY
BIOCHEM-505 4 (2+2)

BLOCK: 2 UNIT-1
PRINCIPLE & APPLICATION OF OF IR AND FTIR SPECTROSCOPY

Dr. ALKA KATIYAR
Teaching Associate

DEPARTMENT OF AGRICULTURAL BIOCHEMISTRY

C.S. AZAD UNIVERSITY OF AGRICULTURE & TECHNOLOGY, KANPUR

Block 1: UNIT-1

TOPIC NAME- PRINCIPLE & APPLICATION OF OF IR AND FTIR SPECTROSCOPY

LECTURE NO- 8

OBJECTIVE-

- Introduction of Infra Red Spectroscopy
- Principle of IR & FTIR Spectroscopy
- Instrumentation and Application of Infra Red Spectroscopy

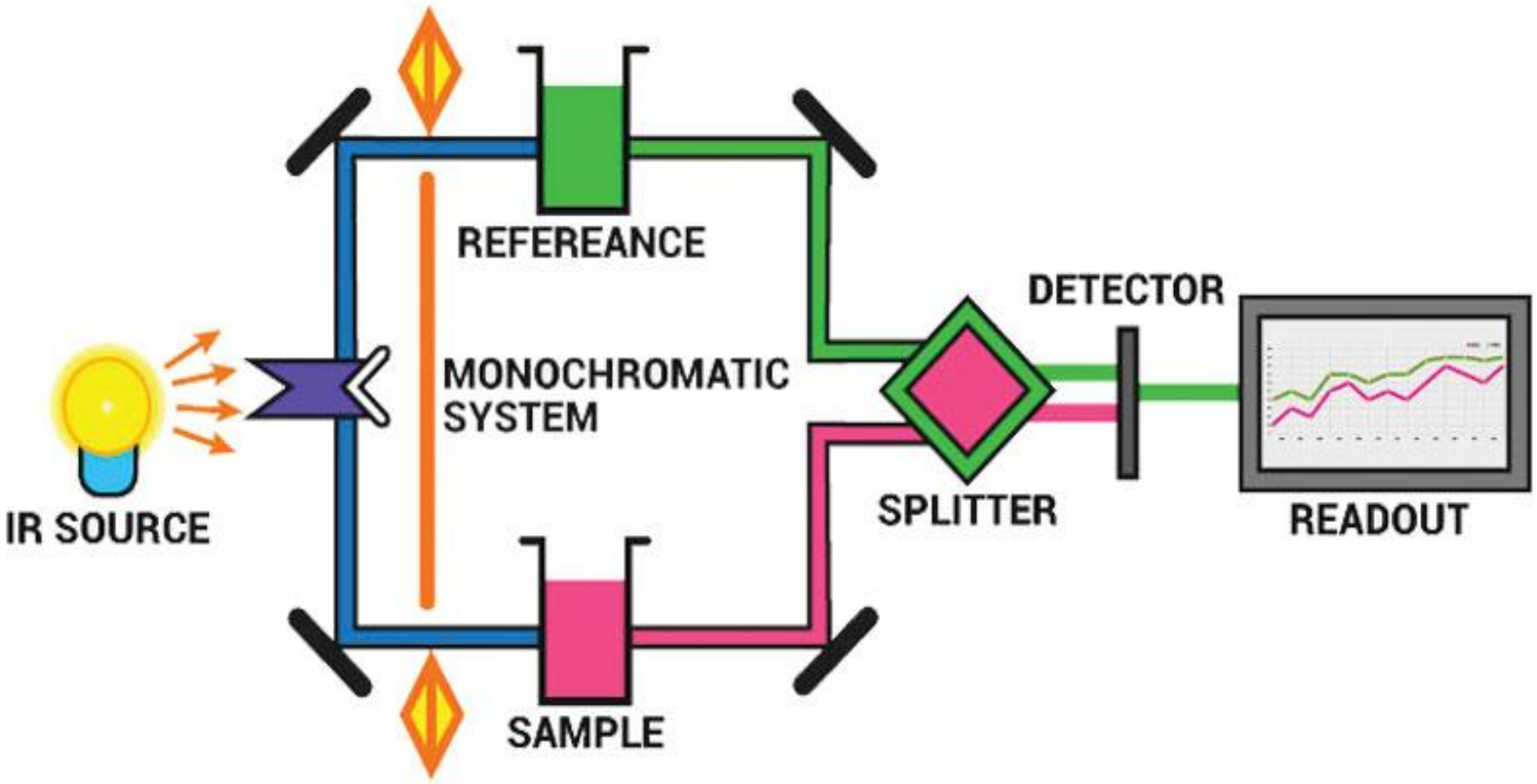
INFRA RED (IR) SPECTROSCOPY

- Infrared (IR) spectroscopy or vibrational spectroscopy is an analytical technique that takes advantage of the vibrational transitions of a molecule.
- It is one of the most common and widely used spectroscopic techniques employed mainly by inorganic and organic chemists due to its usefulness in determining structures of compounds and identifying them.
- The method or technique of infrared spectroscopy is conducted with an instrument called an infrared spectrometer to produce an infrared spectrum.

Principle of Infrared (IR) Spectroscopy

- Infrared Spectroscopy is the analysis of infrared light interacting with a molecule.
- Infrared spectrometers, similar in principle to other spectrometer, permit chemists to obtain absorption spectra of compounds that are a unique reflection of their molecular structure.
- The fundamental measurement obtained in infrared spectroscopy is an infrared spectrum, which is a plot of measured infrared intensity versus wavelength (or frequency) of light.
- IR Spectroscopy measures the vibrations of atoms, and based on this it is possible to determine the functional groups.
- Generally, stronger bonds and light atoms will vibrate at a high stretching frequency

Working of IR Spectroscopy



Instrumentation of Infrared (IR) Spectroscopy

The main parts of IR spectrometer are as follows:-

1. Radiation source
2. Sample cells and sampling of substances
3. Monochromators
4. Detectors
5. Recorder

1.Radiation source

- IR instruments require a source of radiant energy which emit IR radiation which must be steady, intense enough for detection and extend over the desired wavelength.
- Various sources of IR radiations are as follows.

1. Nernst glower
2. Incandescent lamp
3. Mercury arc
4. Tungsten lamp
5. Glober source
6. Nichrome wire

2. Sample cells and sampling of substances

IR spectroscopy has been used for the characterization of solid, liquid or gas samples.

- Solid – Various techniques are used for preparing solid samples such as pressed pellet technique, solid run in solution, solid films, mull technique etc.
- Liquid – Samples can be held using a liquid sample cell made of alkali halides. Aqueous solvents cannot be used as they will dissolve alkali halides. Only organic solvents like chloroform can be used.
- Gas– Sampling of gas is similar to the sampling of liquids.

3. Monochromators

- Various types of monochromators are used such as prism, gratings and filters.
- Prisms are made of Potassium bromide, Sodium chloride or Caesium iodide.
- Filters are made up of Lithium Fluoride and Diffraction gratings are made up of alkali halides.

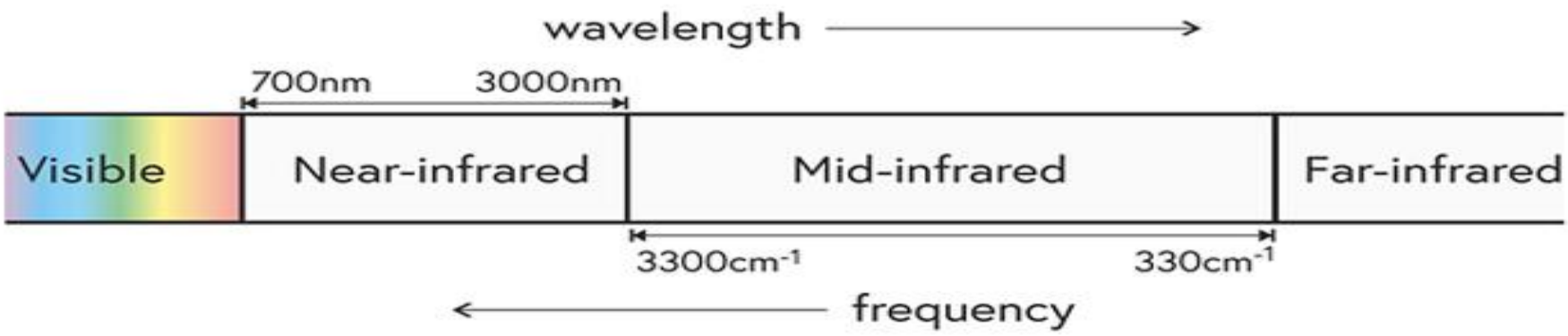
4. Detectors

- Detectors are used to measure the intensity of unabsorbed infrared radiation.
- Detectors like thermocouples, Bolometers, thermisters, Golay cell, and pyro-electric detectors are used.

5. Recorders

- Recorders are used to record the IR spectrum.

Range of IR Spectroscopy are-



$$\text{wavelength} = \frac{\text{speed of light}}{\text{frequency}} \qquad \lambda = \frac{c}{\nu}$$

$$\text{frequency} = \frac{\text{speed of light}}{\text{wavelength}} \qquad \nu = \frac{c}{\lambda}$$

$$\text{wavenumbers} = \frac{\text{frequency}}{\text{speed of light}} \qquad \bar{\nu} = \frac{\nu}{c}$$

Applications of Infrared (IR) Spectroscopy

It has been of great significance to scientific researchers in many fields such as:

1. Protein characterization
2. Nanoscale semiconductor analysis and Space exploration.
3. Analysis of gaseous, liquid or solid samples
4. Identification of compounds
5. Quantitative analysis
6. Information regarding functional groups of molecules and constitution of molecules can be deduced from IR spectrum
7. To know about interaction among molecules

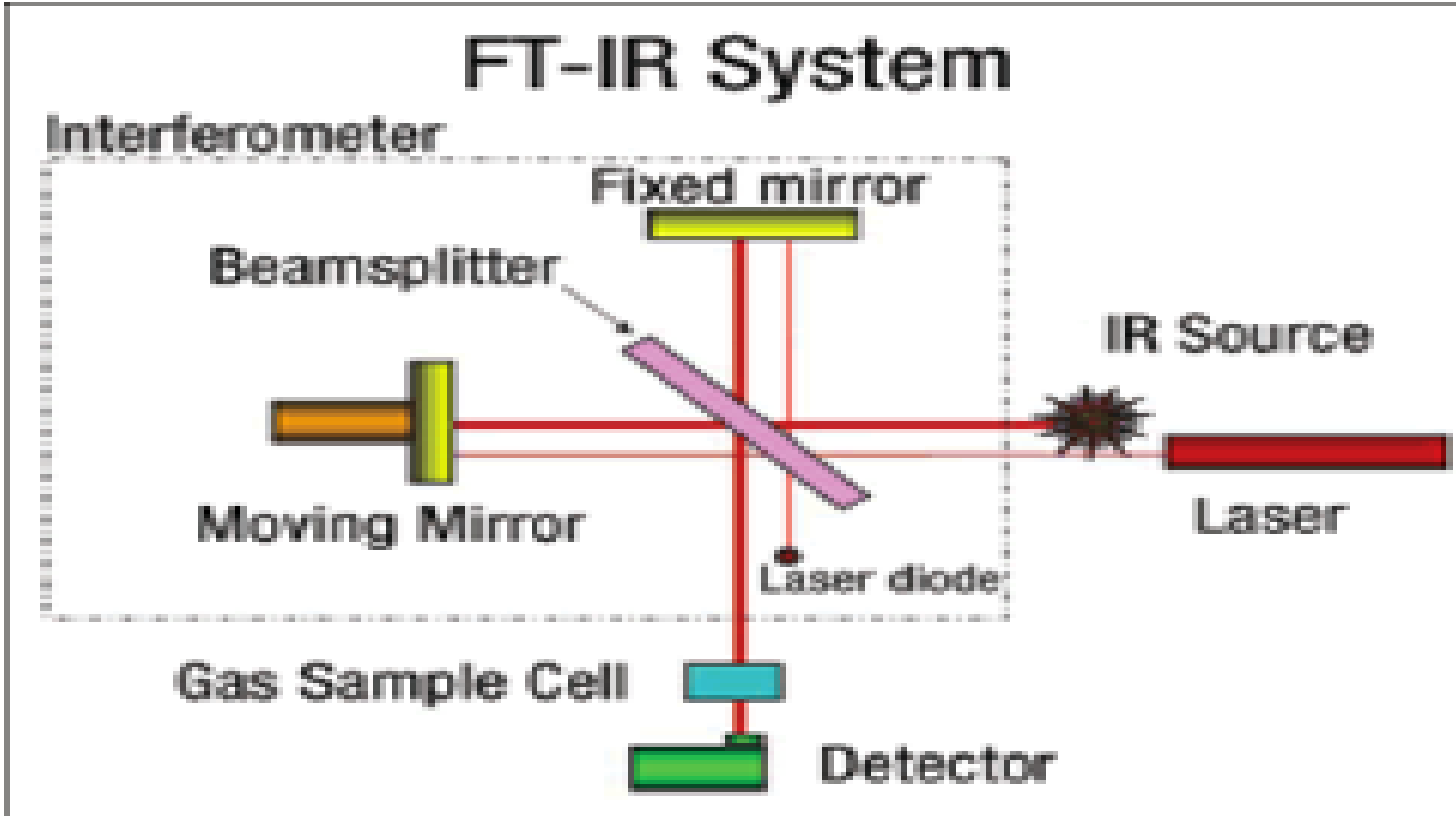
Fourier Transform InfraRed (FTIR)

- FTIR stands for Fourier Transform InfraRed, the preferred method of infrared spectroscopy.
- In infrared spectroscopy, IR radiation is passed through a sample. Some of the infrared radiation is absorbed by the sample and some of it is passed through (transmitted).
- So, what information can FT-IR provide?
- It can identify unknown materials
- It can determine the quality or consistency of a sample
- It can determine the amount of components in a mixture

Why FTIR is important as compared simple IR?

- Fourier transform infrared spectroscopy is preferred over dispersive as well as filter methods of infrared spectroscopy analysis for several reasons:-
- It is a non-destructive technique.
- It provides a precise measurement method which requires no external calibration.
- It can increase speed, collecting a scan every second.
- It can increase sensitivity - one second scans can be co-added together to ratio out random noise.
- It has greater optical output.
- It is mechanically simple with only one moving part.

Working of FTIR-



Application of FTIR Spectroscopy

FTIR applications is extensive. Some of the more common applications are:

- Quality verification of incoming/outgoing materials
- Deformulation of polymers, rubbers, and other materials through thermogravimetric infra-red (TGA-IR) or gas chromatography infra-red (GC-IR) analysis.
- Microanalysis of small sections of materials to identify contaminants
- Analysis of thin films and coatings.
- Monitoring of automotive or smokestack emissions
- Failure analysis

Difference between IR and FTIR Spectroscopy

Sr.no.	Dispersive IR	Fourier Transform IR
1	There are many moving parts resulting in mechanical slippage and wear.	Only the mirror moves during an experiment
2	Calibration against reference spectra is required to measure frequency .	Use of a laser provides high frequency (to 0.01 cm-1).
3	Slow scanning speed.	Rapid scan speeds permit monitoring sample undergoing rapid change.
4	In order to improve resolution only a small amount of the IR beam may be allowed to pass through the slits.	A much larger beam may be used at all times. Data collection is easier .
5	Only radiation of a narrow frequency range falls on the detector at any one time .	All frequencies of radiation fall on the detector simultaniously .
6	The samples is subject to thermal effect from the focused beam .	The sample is not subject to thermal effects.
7	Less sensitive, time consuming.	High sensitivity ,precision & faster .