IR SPECTROSCOPY

ANALYTICAL CHEMISTRY

III B.Sc

SEMESTER – 5

PAPER – 6

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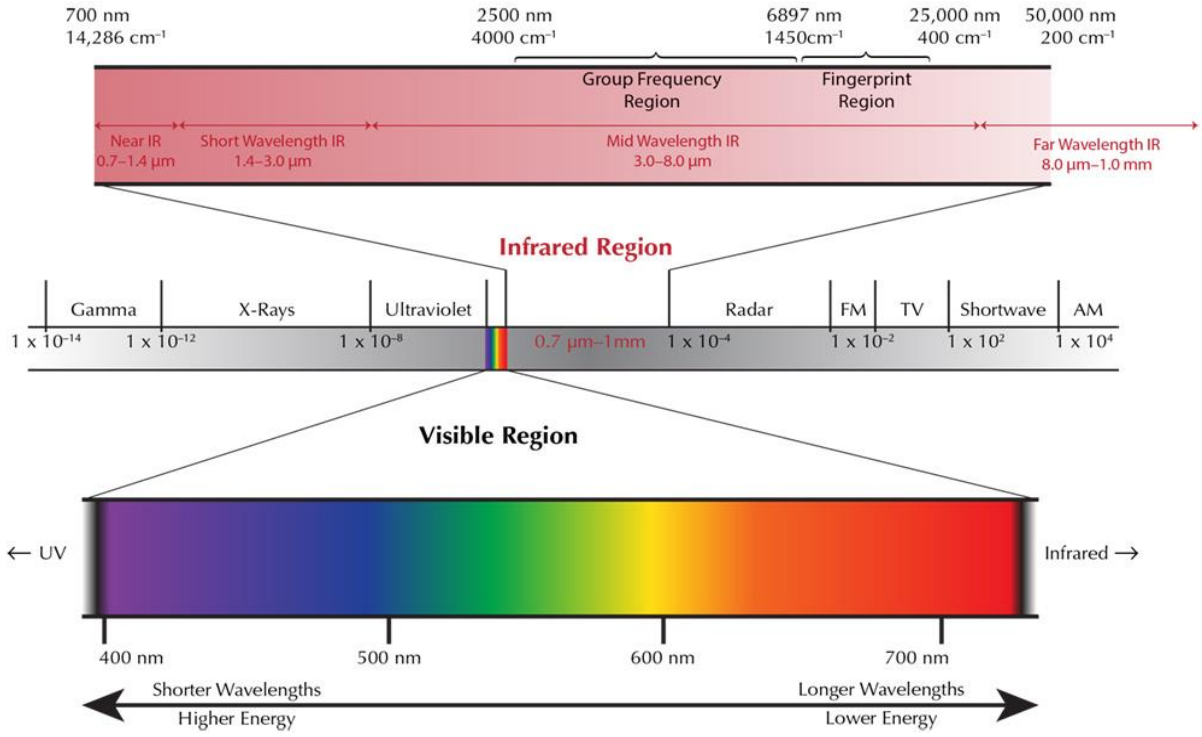
IR SPECTROSCOPY

IR spectroscopy (which is short for infrared spectroscopy) deals with the infrared region of the electromagnetic spectrum, i.e. light having a longer wavelength and a lower frequency than visible light. Infrared Spectroscopy generally refers to the analysis of the interaction of a molecule with infrared light.



The IR spectroscopy concept can generally be analysed in three ways: by measuring reflection, emission, and absorption. The major use of infrared spectroscopy is to determine the functional groups of molecules, relevant to both organic and inorganic chemistry

Regions of the Infrared spectrum:

Most of the bands that indicate what functional group is present are found in the region from 4000 cm^{-1} to 1300 cm^{-1}. Their bands can be identified and used to determine the functional group of an unknown compound.

FUNCTIONAL GROUP REGION	FINGERPRINT REGION
4000 cm^{-1} – 1300 cm^{-1}	1300 cm^{-1} – 400 cm^{-1}

Bands that are unique to each molecule, similar to a fingerprint, are found in the fingerprint region, from 1300 cm^{-1} to 400 cm^{-1}. These bands are only used to compare the spectra of one compound to another.

Principle of Infrared Spectroscopy:

IR spectroscopy works on the principle that molecules absorb specific frequencies that are characteristic of their structure. At temperatures above absolute zero, all the atoms in molecules are in continuous vibration with respect to each other. The IR spectrum of a sample is recorded by passing a beam of IR radiation through the sample.

When the frequency of a specific vibration is equal to the frequency of the IR radiation directed on the molecule, the molecule absorbs the radiation. The examination of the transmitted light reveals how much energy was absorbed at each frequency (or wavelength). Using various sampling accessories, IR spectrometers can accept a wide range of sample types such as gases, liquids, and solids.

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Instrumentation:

The main parts of an IR spectrometer are:

1. IR radiation source.
2. Monochromators
3. Sample cell and sampling of substance.
4. Detector.

1. The IR Radiation Sources:
Infrared instruments need a source of radiant energy which provides a means for isolating narrow frequency band. The radiation source must emit IR radiation which should be:

a. Intense enough for detection
b. Steady.
c. Extend over the desired wavelengths.

The various popular source of IR radiation are as follows

a. Incandescent lamp
b. Nernest glower
c. Globar Source
d. Mercury Arc.

2. Monochromators
The radiation source emits radiation of various frequency as the sample in IR spectroscopy absorb only at certain frequency, it thus becomes essential to select desired frequencies from the radiation source and reject the radiation of other frequencies. Thus, selection has been achieved by means of Monochromators which are mainly of two types:

a. Prism Monochromators
b. Grating Monochromators**.**

3. Sample cells and sampling of substance:

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

i. Solid – Various techniques are used for preparing solid samples such as pressed pellet technique, solid run in solution, solid films, mull technique etc.
ii. 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.
iii. Gas– Sampling of gas is similar to the sampling of liquids.

4. Detector:
The various types of detectors are

a. Bolometers

b. Thermocouples

c. Thermistors

d. Golay cell

e. Photoconductivity cell

Single Beam spectrophotometer:

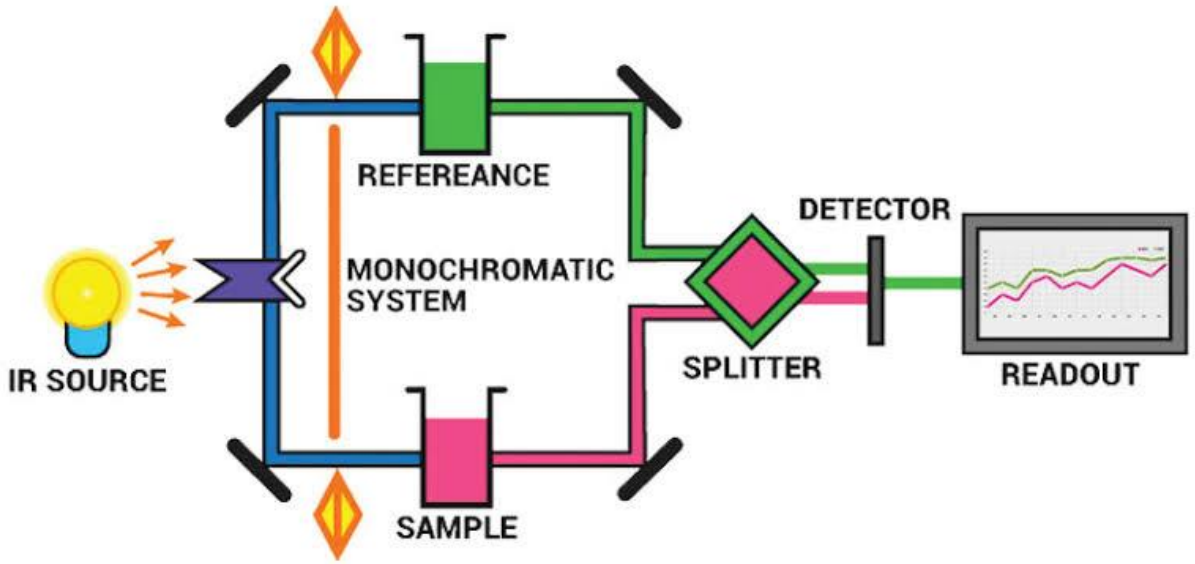
Process
1. In the single – beam system, the radiation is emitted by the source through the sample and then through a fixed prism and rotating Littrow mirror.

2. Both prism and Littrow mirror select the desired wave length and then permit it to pass on to the detector.

3. The detector measures the intensity of radiation after passes through the sample.

4. Knowing the original intensity of radiation, one can measure how much radiation has been absorbed.

5. By measuring the degree of absorption at wavelength, the absorption spectrum of the sample can be obtained.



Application of Infrared Spectroscopy:

1. Identification of substance

2. Determination of Molecular structure

3. Detection of impurities.

4. Isomerism in organic chemistry

5. Identification of functional groups

6. Determination of purity

7. Shape of symmetry of a molecule.

8. Presence of water in a sample.

9. Measurement of paints and varnishes

10. Protein characterization

11. Nanoscale semiconductor analysis

12. Space exploration.

13. Analysis of gaseous, liquid or solid samples

14. Quantitative analysis

15. To know about interaction among molecules