

# Overview of infrared spectroscopy



**ASSIGN  
BUSTER**

Infrared spectroscopy is the most powerful technique used in the analytical laboratory. Infrared spectroscopy is associated with the infrared region.

There are a number of compounds (organic and inorganic), which absorb various frequencies of electromagnetic radiation.

The infrared region is divided into three types; near-IR, mid-IR, and far-IR. In terms of wavelength, the near-IR region extends from  $1400\text{cm}^{-1}$  to  $4000\text{cm}^{-1}$ , mid-IR from  $4000\text{cm}^{-1}$  to  $400\text{cm}^{-1}$  and far-IR from  $400$  to  $10\text{cm}^{-1}$ .

The main function of infrared spectroscopy is to identify all types of organic and inorganic compounds. Functional groups and molecular composition of the compound can also be determined by infrared spectroscopy. It also helps in the quantitative determination of compound mixtures.

In infrared spectroscopy, a molecule absorbs specific frequencies that are characteristic of its structure. This absorption occurs at resonant frequencies, i.e., the frequency of the absorbed radiation matches the frequency of the bond or group that vibrates. In order to absorb IR radiation, a molecule must undergo a net change in dipole moment as a consequence of its vibration.

IR spectra are generally presented in terms of either wavelength or wavenumbers. Wavelength is inversely proportional to the frequency, and wavenumber is directly proportional to the frequency as well as the energy of the IR absorption.

An infrared spectrum is a graph of wavelength versus absorbance (A), but for the IR region, the x-axis is wavenumber (in  $\text{cm}^{-1}$ ) and the y-axis is percent transmittance (%T). Transmittance is the ratio of the radiant power (I) transmitted by a

sample to the radiant power incident on the sample ( $I_0$ ). Absorbance ( $A$ ) is the logarithm to the base 10 of the reciprocal of the transmittance ( $T$ ).

$$A = \log_{10} (1/T) = -\log_{10} T = -\log_{10} I / I_0$$

The transmittance spectra provide better contrast between intensities of strong and weak bands because transmittance ranges from 0 to 100%  $T$  whereas absorbance ranges from infinity to zero. The analyst should be aware that the same sample will give quite different profiles for the IR spectrum, which is linear in wavenumber, and the IR plot, which is linear in wavelength. It will appear as if some IR bands have been contracted or expanded.

## **Molecular vibrations**

The positions of atoms in molecules are not fixed; they are subject to a number of different vibrations. There are two types of vibration;

Stretching: Change in inter-atomic distance along bond axis; there are two types of stretching;

- Asymmetric stretching
- Symmetric stretching

Bending: Change in angle between two bonds. There are four types of bend:

- Rocking
- Scissoring
- Wagging
- Twisting

In the organic molecule each bond having its characteristics stretching and bending frequency and capable of absorbing light of that frequency.

Stretching absorption of a bond appears at higher frequencies in the infrared spectrum than the bending absorptions of the same bond.

The position of absorption bands depends on the relative masses of the atoms, the force constants of the bonds and the geometry of the atom.

The HOOKE' S law, which gives frequency with bond strength and atomic masses, since

For a diatomic molecule A-B, the wavenumber (in  $\text{cm}^{-1}$ ) of the absorption ;

There are two useful regions in the IR spectrum. The group frequency region encompasses 3600 to 1200  $\text{cm}^{-1}$  region, where the identical functional groups fingerprint region from 1200 to 700  $\text{cm}^{-1}$  and it reflects the absorptions from the skeletal structure of the molecule. Small differences in the structure result in significant changes in fingerprint region so it leads to great evidence for the identity of the compounds yielding the spectra. Only stereoisomers absorb exactly in the same way in this region.

There are several instrument used to determine the absorption for a compound is called an infrared spectrometer. There are two types of infrared spectrometer;

Dispersive infrared spectrometer

Fourier transfer infrared spectrometer (FT-IR)

Both the instrument measures the spectra of the compounds in the range of 4000 to 400 $\text{cm}^{-1}$ .

Now a day, number of industries and laboratories worked on the FT-IR.

Because dispersive infrared spectrometer has many limitation, like it suffer from sensitivity, speed and wavelength accuracy. FT-IR gives infrared spectrum within a second. The main advantage of use of FT-IR is that FT-IR does not have the slits. This is present in the dispersive infrared. Because the some of the light is pass through the slit, so there is loss of light.

## **Fourier transfer infrared spectrometer (FT-IR)**

The main components of the FT-IR are radiation source, interferometer and detector.

Source :-

The sources are rod in shape. They are heated by electronically around 1800 oc. The sources rods are made up from the Nernst glower (Zr, Th, Ce, Er, etc), Globar (silicon carbide) an other ceramic materials.

The light comes from these sources are passed through the interferometer.

The interferometer is a design in which two optical paths gets divided and then recombines them and produce wave type pattern, which contain all the frequencies. Those form the infrared spectrum.

Interferometer

The interferometer used in the FT-IR is called as the Michelson interferometer.

Michelson interferometer consist three basic components; moving mirror, fixed mirror and Beam splitter.

The beam splitter is a semi reflecting device and is often made by depositing a thin film of germanium onto a flat KBr substrate. The light comes from the sources and its strikes on beam splitter. Which is designed to split the beam (A) exactly in half.

The beam (B) is transmitted towards fixed mirror and its get reflected back towards the beam splitter, other beam (C) is transmitted towards moving mirror and it's also get reflected back towards the beam splitter. Both the beam is recombine at the beam splitter and high intensity radiation will reach the detector.

Fig:- Michelson interferometer

Michelson interferometer an optical path difference is introduced between the two beams by translating the moving mirror away from the beam splitter. A general property of (optical) waves is that their amplitudes are additive. When the beams that have reflected off the fixed and moving mirrors recombine at the beam splitter are in phase, an intense beam leaves the interferometer as a result of constructive interference. When the fixed and moving mirrors beams are recombined at the beam splitter and the waves are completely out of phase, a low intensity beam leaves the interferometer as a result of destructive interference. The sample is placed between the source and the beam splitter.

Detectors

In the FT-IR to get the good sensitivity and speed in recording the spectrum must be matched in the speed and photometric accuracy of the detectors; this is achieved by thermal detectors based on pyroelectric materials or on solid state semiconductor devices based on photovoltaic or photoconductive principles.

The main advantages of an FT-IR instrument is that it collect dozens of interferogram of the sample and accumulate them in the memory of a computer. To obtain a spectrum of a compound, the chemist first obtain an interferogram of the background which consists of the infrared-active atmospheric gases, carbon dioxide and water vapour (oxygen and nitrogen are not infrared active). The interferogram is subjected into a Fourier transform, which yield the spectrum of the background. Then the chemist places the compound (sample) and obtains the spectrum resulting from the Fourier transform of the interferogram. This spectrum contains absorption bands for both the compound and background. The computer software automatically subtracts the spectrum of the background from the sample spectrum, and the obtain spectrum of the compound being analyzed.

An infrared spectrometer determines the position and relative sizes of all the absorptions, or peaks, in the infrared region and plots them on a piece of paper. The spectrum gives at least two strongly absorbing peaks at about 3000 and 1715  $\text{cm}^{-1}$  for the C-H and C=O stretching frequencies respectively. The given table show the frequency of the different functional group to identify the peaks of the band, which obtain in the spectrum.