IR Spectroscopy

Introduction

IR spectroscopy or infrared spectroscopy is also called as vibrational spectroscopy. It implicates an interaction of infrared radiation with matter. Absorption spectroscopy techniques are covered in it and are used to recognize chemicals and study chemicals. An infrared spectrometer is a tool with which the infrared spectroscopy can be done, an infrared spectrometer is also called as a spectrophotometer and is availed to generate an infrared spectrum.

The infrared spectrum is fundamentally a graph which has thefrequency on a horizontal axis or else wavelength on the horizontal axis and infrared light absorbance on vertical axis. Reciprocal centimeters or wave numbers are the units of frequency availed in IR spectra. The microns or micrometers are units used to represent IR wavelength. A usual equipment of laboratory which avails this method is a Fourier transform infrared spectrometer and also called as FTIR spectrometer.

Definition

Infrared spectroscopy (IR) is a characterization tool chemists use to help determine the molecular structure. IR capitalizes on the concept that functional groups absorb specific frequencies of energy based on their structure. When a functional group absorbs energy, it can vibrate in a bending or stretching mode and the characteristic energy for this vibrational mode is reported in wavenumbers.

A change in molecular dipole is required for a bending or stretching mode to be visible in by IR. In general, stronger bonds vibrate at higher wavenumbers, as do bonds between atoms of very different size. IR is a reliable and sensitive technique that has important applications in crime-scene investigation, for example in solving a case of arson, IR can identify traces of fuel or accelerant.

Applications of IR Spectroscopy

Infrared spectroscopy is widely used in industry as well as in research. It is a simple and reliable technique for measurement, quality control and dynamic measurement. It is also employed in forensic analysis in civil and criminal analysis.

Some of the major applications of IR spectroscopy are as follows:

1. Identification of functional group and structure elucidation

Entire IR region is divided into group frequency region and fingerprint region. Range of group frequency is 4000-1500 cm^{-1} while that of finger print region is 1500-400 cm^{-1}.

In group frequency region, the peaks corresponding to different functional groups can be observed. According to corresponding peaks, functional group can be determined.

Each atom of the molecule is connected by bond and each bond requires different IR region so characteristic peaks are observed. This region of IR spectrum is called as finger print region of the molecule. It can be determined by characteristic peaks.

2. Identification of substances

IR spectroscopy is used to establish whether a given sample of an organic substance is identical with another or not. This is because large number of absorption bands is observed in the IR spectra of organic molecules and the probability that any two compounds will produce identical spectra is almost zero. So if two compounds have identical IR spectra then both of them must be samples of the same substances.

IR spectra of two enatiomeric compound are identical. So IR spectroscopy fails to distinguish between enantiomers.

For example, an IR spectrum of benzaldehyde is observed as follows.

C-H stretching of aromatic ring- 3080 cm^{-1}

C-H stretching of aldehyde- 2860 cm^{-1} and 2775 cm^{-1}

C=O stretching of an aromatic aldehyde- 1700 cm^{-1}

C=C stretching of an aromatic ring- 1595 cm^{-1}

C-H bending- 745 cm^{-1} and 685 cm^{-1}

No other compound then benzaldehyde produces same IR spectra as shown above.

3. Studying the progress of the reaction

Progress of chemical reaction can be determined by examining the small portion of the reaction mixure withdrawn from time to time. The rate of disappearance of a characteristic absorption band of the reactant group and/or the rate of appearance of the characteristic absorption band of the product group due to formation of product is observed.

4. Detection of impurities

IR spectrum of the test sample to be determined is compared with the standard compound. If any additional peaks are observed in the IR spectrum, then it is due to impurities present in the compound.

5. Quantitative analysis

The quantity of the substance can be determined either in pure form or as a mixure of two or more compounds. In this, characteristic peak corresponding to the drug substance is chosen and log I0/It of peaks for standard and test sample is compared. This is called base line technique to determine the quantity of the substance.

Advantages & Disadvantages of Infrared Spectroscopy

Infrared spectroscopy is when an instrument uses infrared radiation to detect through "mechanical sight" things that may be difficult to see in other spectra. For instance, hydrocarbons can be detected through infrared spectroscopy. While using this process has a number of advantages, it also has some disadvantages.

Non-Destructive

One of the primary advantages is that infrared spectroscopy causes no damage. Several other forms of mechanical sight can detect particles through other spectra, but many of their methods use radiation. For example, X-ray technology requires precautions so that the radiation doesn't cause damage to people in the area. However, infrared radiation is harmless and won't damage the environment or the area being viewed.

Sensitivity

One downside of using infrared spectroscopy is that it requires very sensitive and properly tuned instruments. Any basic infrared instrument can see the infrared spectrum, but being able to focus on it well enough to make sense of what's being seen requires tools that are well tuned. Also, the better tuned and focused a set of tools happens to be, the more expensive it will be to buy and maintain in the long term.

Preparation

A major advantage of infrared spectroscopy is that the samples being viewed don't require any sort of special preparation. Some tests may require a subject to be bathed in radiation or have radioactive dye put into it, but infrared spectroscopy doesn't require that. The detection instruments simply need to be set up so they can "look" at the subject. The readings can be taken without doing anything special to the subject at hand.

Conclusion

IR identifies the components of a sample (liquid, solid or gas). Infrared (IR) spectrometers measure the interaction of IR radiation with samples. The FTIR spectrometer measures the frequencies at which the samples absorb the radiation, and the intensities of the absorptions. Intensity and frequency of samples absorption are depicted in a two-dimensional plot called a spectrum.

Intensity is generally reported in terms of absorbance - the amount of light absorbed by a sample, or percent transmittance – i.e. the amount of light, which passes through it. What makes up an unknown sample, and how much of each component is present in that sample, can be valuable information supplied by this technique. Its many applications include research and development of new products.