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Application of Infra-Red Spectroscopy to the Determination of Inorganic Compounds

Sandeep Kumar*

Assistant Professor, Department of Chemistry, Government College, Narnaund

Abstract* – *Spectroscopy can be defined as the interaction between matter and light. Infrared spectroscopy is a very powerful technique which uses electromagnetic radiation in the infrared region for the determination and identification of molecular structure as well as having various quantitative applications within analytical chemistry.

Infrared spectroscopy is the study of the interaction of infrared light with matter. 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.

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INTRODUCTION

Infrared spectrometers use optical devices for dispersing and focusing electromagnetic radiation of IR frequency which is passed through the sample and any changes in absorbance measured against a reference beam. There are three well defined IR regions (near, mid and far). The boundaries between them are not clearly defined and debate still persists, but broadly they are defined as:

- Near infrared (12820-4000 cm-1): poor in specific absorptions, consists of overtones and combination bands resulting from vibrations in the mid-infrared region of the spectrum.

- Mid-infrared (4000-400 cm-1): provides structural information for most organic molecules.

- Far Infrared (400-33 cm-1): has been less investigated than the other two regions; however, it has been used with inorganic molecules.

INFRARED SPECTROSCOPY

Infrared spectroscopy can be rationalized as the spectroscopy that deals with electromagnetic radiation of infrared frequency. As previously explained, there are three well defined infrared regions; each of them has the potential to provide different information:

Far-Infrared (400-33 cm-1): vibrations of molecules containing heavy atoms, molecular skeleton vibrations and crystal lattice vibrations

Mid-Infrared (4000-400 cm-1): useful for organic analysis

Near Infrared (12820-4000 cm-1): overtones; very useful for quantitative analysis Infrared spectroscopy is one of the most useful and widely used methods to perform structural analysis.

Infrared spectroscopy exploits the fact that molecules absorb specific frequencies that are characteristic of their structure. These absorptions are resonant frequencies, i.e. the frequency of the absorbed radiation matches the frequency of the bond or group that vibrates. The energies are determined by the shape of the molecular potential energy surfaces, the masses of the atoms, and the associated vibronic coupling.

In particular, in the Born-Oppenheimer and harmonic approximations, i.e. when the molecular Hamiltonian corresponding to the electronic ground state can be approximated by a harmonic oscillator in the neighborhood of the equilibrium molecular geometry, the resonant frequencies are determined by the normal modes corresponding to the molecular electronic ground state potential energy surface. Nevertheless, the resonant frequencies can be in a first approach related to the strength of the bond, and the mass of the atoms at either end of it. Thus, the frequency of the vibrations can be associated with a particular bond type.

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.

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Corresponding Author

Sandeep Kumar*

Assistant Professor, Department of Chemistry, Government College, Narnaund