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Applications of Infra-Red Spectroscopy

Ganga Shy Meena

Assistant Professor, Department of Chemistry, Government College, Sawai Madhopur, Rajasthan, India

ABSTRACT

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 analyzed 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.

KEYWORDS: *IR spectroscopy, electromagnetic, alkanes, applications, reflection, emission, absorption, functional, structure, range*

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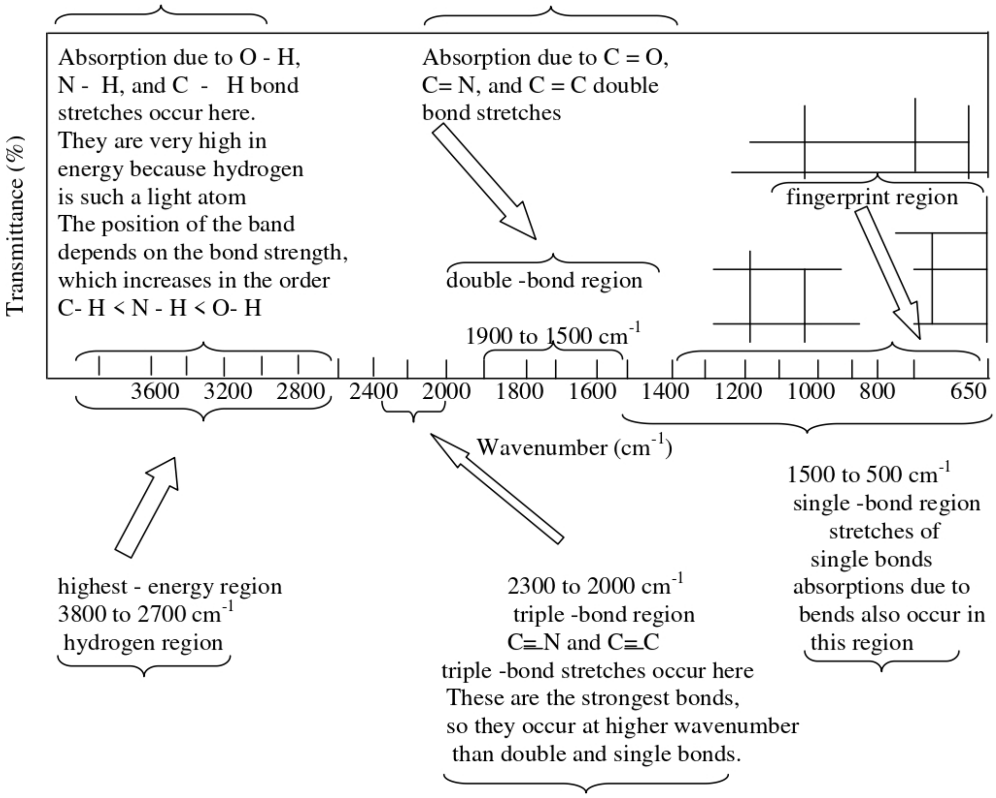
INTRODUCTION

Infra-red spectrum of a compound provides more information than is normally available from the electronic spectra. In this technique, almost all groups absorb characteristically within a definite range. The shift in the position of absorption for a particular group may change (within the range) with the changes in the structure of the molecule. [1,2]

Characteristic Group Frequencies of organic Molecules



1. Alkane

C-H stretching is most characteristic of alkanes, C-H bending is also sighificant C-H stretching appear in the range of 2960-2850 Cm^{-1} (m,s).

Methyl group shows two distinct bands at 2962 Cm^{-1} and 1872 Cm^{-1} for asymmetric and symmetric stretching mode respectively. methyelene group have asymmetric stretching at 2926 Cm^{-1}

and symmetric stretching at 2853 Cm^{-1}.The bending vibration of methyl group and methyelne group occur at 1380Cm^{-1} and 1465 Cm^{-1}

The band resulting from methyelene rocking vibration appears at 720 Cm^{-1}.

2. Alkene

C=C H str. - 3100-3000Cm^{-1}

C=C stretching vibration show medium absorption band at 1680-1460Cm^{-1} absorption frequency of C=C is reduced by about 30Cm^{-1}due to conjugation.

R-CH=CH_2	C_6H_5-CH=CH2	=CH_2
1640	1625	(all in Cm^{-1})

Olefinic C-H stretching vibration band occurs around 3080 Cm^{-1}, which is also the region of aromatic C-H stretching. The Characteristic of olefins is out of Plane C-H bending at 1000-650Cm^{1}.

3. Alkynes

Alkynes have two stretching modes:

C≡C stretch at 2260-2100 Cm^{-1}.

≡ C-H stretch at 3300Cm^{-1}.

C-H bending vibration of alkyne occurs at 700-610 Cm^{-1} In internal alkyne (R-C≡C-R) C≡C stretch may be very weak or absent due to small or no change in dipole moment. [3,4]

4. Aromastic hydrocarbon

A. Aromatic C-H stretch occur at 3050-3000Cm^{-1}
B. Overtone appears at 2000-1650Cm^{-1}
C. C-C ring stretch occur at 1600, 1580, 1500, 1450 Cm^{-1}Vibration frequency is lowered due to conjugation.
D. Out of plance C-H band at below 900Cm^{-1}. This spectra is most infomative.

5. Alcohol and phenol

O-H stretching & C-O stretching are characteristic stretching. If OH is free then sharp absorption occur at=3600 Cm^{-1}. Such absorption occurs only in vapour phase or in dilute solution of alcohol in non-polar solvent. In the presence of H-bonding an intense broad peak appear at=3600 Cm^{-1}.

Due to steric hindrance this compound does not have h bonding so-OH stretch occur at 3600Cm^{-1}.

C-O stretching vibration in alcohol produces at 1260-1050Cm^{-1}frequency of this band is used to distinguish between primary, secondary, and tertiaary alcohol.

6. Ether

The characteristic of ether is strong C-O stretching band at 1050-1275Cm^{-1}. In case of highly asymmetrical ethers e.g. alkyl aryl ether the two C-O band couple and show two bands for asymmetric and symmetric stretching.

7. Carbonyl group

The carbonyl group can be recognized by a strong absorption around 1850-1660Cm^{-1}.

The carbonyl group forms parts of various group such aldehydes, ketone, acid, acid chloride, anhydride, ester, acid amide, lactone, alctum etc.

A. Aldehydes:

Aldehydes show C=O stretching at 1730-1725 Cm^{-1}. If electronegative atom is attached to α carbon of aldehydes then it increases the frequency of $v_{c=o}$. For example.

CH_3-CHO	Cl_3C-CHO	
1730	1768	(all in Cm^{-1})

In α,β unsaturated aldehydes conjugation decreases the $v_{c=o}$. freauency. for example,

CH_3-CHO	CH_3-CH_2=CH-CHO
1730	(all in Cm^{-1})

CH stretching occurs at 2825Cm^{-1}, 2720Cm^{-1} as a doublet due to fermi resonance with overtone of C-H bending at 1390Cm^{-1}.

B. Ketones:

ketones show C=O stretching near at 1715Cm^{-1}. as aldehydes conjugation decreases the vibration frequency of C=O bond also decreases.

8. Carboxylic acids:

O-H stretching frequency in the solid & Pure liquid occurs at 3300-2500Cm^{-1} as broad strong absorption due to H-bonding. C=O stretching bands occurs at 1725-1700Cm^{-1}. This due to electron donating nature of – OH group (+M>-I). C-O stretching occurs at 1320-1210Cm^{-1}.

9. Esters:

C=O stretching bands occurs at 1750-1735 Cm^{-1}. Conjugation reduced the double bond character of C=O group so vibration frequency decreases. so $v_{c=o}$ of Benzoate ester is 1715 Cm^{-1}.

10. Acid halides:

R-CO-X, where X=F, Cl, Br, I. $v_{c=o}$= 1815-1785 Cm^{-1}. Since halide have – I effect greater than +M effect so C=O stretching frequency is greater than carbony compounds.

11. Acid anhydride:

Anhydride displays two stretching bands due to coupled asymmetric & Symmetric stretching mode of C=O group occurs at 1850-1800 Cm^{-1} and 1790-1740 Cm^{-1}.[5,6]

12. Amides:

All amides show C=O stretching band at 1700-1650Cm^{-1}, this band is known as amide I-band. Primary and secondary amides show N-H bending in the region 1650-1510Cm^{-1}. This is known as amide II band. All amides display C-N stretching band at 1300-1050Cm^{-1}, known as amide III band.

Primary amide show doublet at 3500-3400Cm^{-1} due to coupled N-H stretching. Secondary amides show singlet at near 3400 Cm^{-1} due to N-H H-Amines stretching.

13. Compounds containing nitrogen:

(a). Nitro compounds: These compounds show two very intense absorphtion bands in the 1560-1500Cm^{-1} and 1350-1300Cm^{-1}. region of the speotrum due to asymmetric and symmetric stretcning vibrations of the highly polar nitrogen-orygen bonds. Aromatic nitro compounds show hands at slightly lowe freauencies then the aliphatic compounds because of a conjugation of the intro grup with the aromatic ring. which slightly weakens the nitrogen-orygen bonds.

(b). Nitroso compounds: These Compounds may represent C-NO or N-NO type. Tertiary C-nitroso compouns tend to dimerise, and secondary and primary C-nitroso compounds readily rearrang to oximes. In the monomaric state they absorb in the 1600-1500Cm^{-1}–egion, howver, in solution they exist preferentially as dimers and then absorb near 1290Cm^{-1}(cis) or 1400Cm^{-1}(trans).

N-Nitroso compounds show a band near 1450Cm^{-1}in ccl_4solution.

(c). Nitrites: These Compounds display their N=o stretching vibration as two bands near 1660$Cm^{-1}$and 1620Cm^{-1}, these are attributed to the trans and cis forms of the nitrite[7,8]

14. Hetro aromatic Compounds:

Hetroaromatics such as pyridine, furan, thiophene etc. show C-H str bands in the region 3077-3000Cm^{-1}. such compounds containing N-H group show N-H str absorption in the region 3500-3220Cm^{-1}. In this region of absorption, the exact position depends upon the degree of hydrogen bonding and hence upon the physical state of the sample or the polarity of the solvent. Pyrrole and Indole in dilute solution in noon-polar solvents show a sharp bands near 3495Cm^{-1}.

Ring stretching vibrations occur in the general region between 1600-1300Cm^{-1}. The absorption involves stretching and Contraction of all the bonds in the ring and interaction between these stretching modes.

15. Amines: Amines are the alkyl derivatives of ammonia. These can be recognised by absorption due to N-H str in the region 3500-3300Cm^{-1}. The position of absorption depends upon the degree of hydrogen bonding. Primary amines show two sharp bands; secondary amines give only one band while tertiary amines do not absorb in the said N-H str region. N-H and O-H groups have some common properties and their absorption due to these group are superimposed making their identification difficult.

Since nitrogen atom is less electronegative than oxygen atom, the N-H…N hydrogen bonds are weaker as compared to O-H…O bonds and hence frequency shifts due to hydrogen bonding in amine are smaller V^N-H absorption occur at lower freauencies amine in an inert solvent give two sharp bands due to asymmetric stretching vibvations between 3500-3300Cm^{-1}.[9,10]

Discussion

An IR spectrum is essentially a graph plotted with the infrared light absorbed on the Y-axis against. frequency or wavelength on the X-axis. An illustration highlighting the different regions that light can be classified into is given below.

IR Spectroscopy detects frequencies of infrared light that are absorbed by a molecule. Molecules tend to absorb these specific frequencies of light since they correspond to the frequency of the vibration of bonds in the molecule.

The energy required to excite the bonds belonging to a molecule, and to make them vibrate with more amplitude, occurs in the Infrared region. A bond will only interact with the electromagnetic infrared radiation, however, if it is polar.

The presence of separate areas of partial positive and negative charge in a molecule allows the electric field component of the electromagnetic wave to excite the vibrational energy of the molecule.

The change in the vibrational energy leads to another corresponding change in the dipole moment of the given molecule. The intensity of the absorption depends on the polarity of the bond. Symmetrical non-polar bonds in N≡N and O=O do not absorb radiation, as they cannot interact with an electric field.

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.[11,12]

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.

The samples used in IR spectroscopy can be either in the solid, liquid, or gaseous state.

- Solid samples can be prepared by crushing the sample with a mulling agent which has an oily texture. A thin layer of this mull can now be applied on a salt plate to be measured.
- Liquid samples are generally kept between two salt plates and measured since the plates are transparent to IR light. Salt plates can be made up of sodium chloride, calcium fluoride, or even potassium bromide.
- Since the concentration of gaseous samples can be in parts per million, the sample cell must have a relatively long pathlength, i.e. light must travel for a relatively long distance in the sample cell.

Thus, samples of multiple physical states can be used in Infrared Spectroscopy.

Results

The IR spectroscopy theory utilizes the concept that molecules tend to absorb specific frequencies of light that are characteristic of the corresponding structure of the molecules. The energies are reliant on the shape of the molecular surfaces, the associated vibronic coupling, and the mass corresponding to the atoms. For instance, the molecule can absorb the energy contained in the incident light and the result is a faster rotation or a more pronounced vibration.

Now, both of these beams are reflected to pass through a splitter and then through a detector. Finally, the required reading is printed out after the processor deciphers the data passed through the detector. IR spectroscopy involves the collection of absorption information and its analysis in the form of a spectrum

By using computer simulations and normal mode analysis it is possible to calculate theoretical frequencies of molecules.

A spectrograph is often interpreted as having two regions.

- **functional group region**

In the functional region there are one to a few troughs per functional group.

- **fingerprint region**

In the fingerprint region there are many troughs which form an intricate pattern which can be used like a fingerprint to determine the compound.

Conclusions

Infrared spectroscopy is a simple and reliable technique widely used in both organic and inorganic chemistry, in research and industry. In catalysis research it is a very useful tool to characterize the catalyst, as well as to detect intermediates and products during the catalytic reaction. It is used in quality control, dynamic measurement, and monitoring applications such as the long-term unattended measurement of CO2 concentrations in greenhouses and growth chambers by infrared gas analyzers. It is also used in forensic analysis in both criminal and civil cases, for example in identifying polymer degradation. It can be used in determining the blood alcohol content of a suspected drunk driver.IR-spectroscopy has been successfully used in analysis and identification of pigments in paintings and other art objects such as illuminated manuscripts.[13]

A useful way of analyzing solid samples without the need for cutting samples uses ATR or attenuated total reflectance spectroscopy. Using this approach, samples are pressed against the face of a single crystal. The infrared radiation passes through the crystal and only interacts with the sample at the interface between the two materials. With increasing technology in computer filtering and manipulation of the results, samples in solution can now be measured accurately (water produces a broad absorbance across the range of interest, and thus renders the spectra unreadable without this computer treatment).Some instruments also automatically identify the substance being measured from a store of thousands of reference spectra held in storage.

Infrared spectroscopy is also useful in measuring the degree of polymerization in polymer manufacture. Changes in the character or quantity of a particular bond are assessed by measuring at a specific frequency over time. Modern research instruments can take infrared measurements across the range of interest as frequently as 32 times a second. This can be done whilst simultaneous measurements are made using other techniques. This makes the observations of chemical reactions and processes quicker and more accurate. Infrared spectroscopy has also been successfully utilized in the field of semiconductor microelectronics: for example, infrared spectroscopy can be applied to semiconductors like silicon, gallium arsenide, gallium nitride, zinc selenide, amorphous silicon, silicon nitride, etc. Another important application of Infrared Spectroscopy is in the food industry to measure the concentration of various compounds in different food products. The instruments are now small, and can be transported, even for use in field trials.

Infrared Spectroscopy is also used in gas leak detection devices such as the DP-IR and Eye CGAs. These devices detect hydrocarbon gas leaks in the transportation of natural gas and crude oil. In February 2014, NASA announced a greatly upgraded database, based on IR spectroscopy, for tracking polycyclic aromatic hydrocarbons (PAHs) in the universe. According to scientists, more than 20% of the carbon in the universe may be associated with PAHs, possible starting materials for the formation of life. PAHs seem to have been formed shortly after the Big Bang, are widespread throughout the universe, and are associated with new stars and exoplanets. Infrared spectroscopy is an important analysis method in the recycling process of household waste plastics, and a convenient stand-off method to sort plastic of different polymers (PET, HDPE, ...).

Other developments include a miniature IR-spectrometer that's linked to a cloud based database and suitable for personal everyday use, and NIR-spectroscopic chips that can be embedded in smartphones and various gadgets.[14]

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