Journal for Research in Applied Sciences and Biotechnology
www.jrasb.com

ISSN: 2583-4053
Volume-2 Issue-5 || October 2023 || PP. 128-131
https://doi.org/10.55544/jrasb.2.5.21

Determining of Chemical Bond Properties in Hydrocarbons by Using Infrared Spectrum

Puhandoy Amir Mohammad Khair Oghli
Department of Chemistry, Faculty of Medical, Balkh University, AFGHANISTAN.

Corresponding Author: akhairoghli@gmail.com

www.jrasb.com || Vol. 2 No. 5 (2023): October Issue

Received: 11-10-2023 **Revised:** 21-10-2023 **Accepted:** 31-10-2023

ABSTRACT

The spectroscopy of infrared is type of vibrational spectroscopy which is bases on the fact that a molecule absorbs infrared radiation, it is chemical bond vibrate. The bonds can stretch, contract, and bend have characteristic vibrations depending on the atoms in the bond, the number of bonds, and the orientation of those bonds with respect to the rest of the molecule. The troughs in the spectrum are caused by the absorption of infrared frequencies by chemical bonds, which are often characteristic of combinations of atoms or functional groups.

The light of infrared can create the bond angle between the atoms in a compound to decrease and increase as it reaches back to equilibrium. While a molecule of a compound absorbs the light of infrared radiation, its chemical bonds vibrate. When the radiation is absorbed, the bond can stretch, contract, and bend. This is the reason that the infrared spectroscopy is a type of vibrational spectroscopy. When the bond absorbs the radiation that matches the frequency of the vibration of one of its bonds and this means that the molecule is exposed to infrared radiation.

The radiation of infrared absorbed allows the bond to vibrate a bit more, that is increase the amplitude observation, but the vibrational frequency will remain the same.

Keywords- Radiation, Frequency, Light, Spectroscopy, wave and electromagnetic.

I. INTRODUCTION

Almost any compound having covalent bonds, whether organic or inorganic, absorbs various frequencies of electromagnetic radiation in the infrared region of the electromagnetic spectrum. This region lies at wavelengths longer that those associated with visible light, which range from approximately 400 to 800 nm, but lies at wavelengths shorter that those associated with microwaves, which are longer that 1mm. for chemical purposes, we are interested in the vibrational portion of the infrared region [10]. It includes radiation with wavelengths between 2.5 µm and 25 µm (1 µm = 10^{-6} m). Although the more technically correct unit for wavelength in the infrared region of the spectrum is the micrometer (µm), you will often see the micron (µ) used on infrared spectra.

When a molecule absorbs infrared radiation, its chemical bonds vibrate [4]. The firs necessary condition for a molecule absorb infrared light is that the molecule must have a vibration during which the change in dipole moment with respect to distance in non-zero. This condition can be summarized in equation form as follows:

$$\frac{\partial\mu}{\partial x} \neq 0 \qquad \begin{array}{l} \partial\mu = \text{change in dipole moment} \\ \partial x = \text{change in bond distance} \end{array}$$

The vibrations that satisfy this equation are called to be infrared active. The H-Cl stretch of hydrogen chloride and the asymmetric stretch of CO_2 are examples of infrared active vibration. Infrared active vibrations cause the bands seen in an infrared spectrum [1].

Secondly the necessary condition for infrared absorbance is that the energy of the light impinging on a molecule must equal a vibration energy level difference within the molecule. This condition can be summarized in equation as follows:

$$\Delta E_{vib} = hcW$$

ΔE_{vib} = vibrational energy level difference in a molecule
h = Planck's Constant (Joule-sec)
c = the speed of light (cm/sec)
W = wavenumber in cm^{-1}

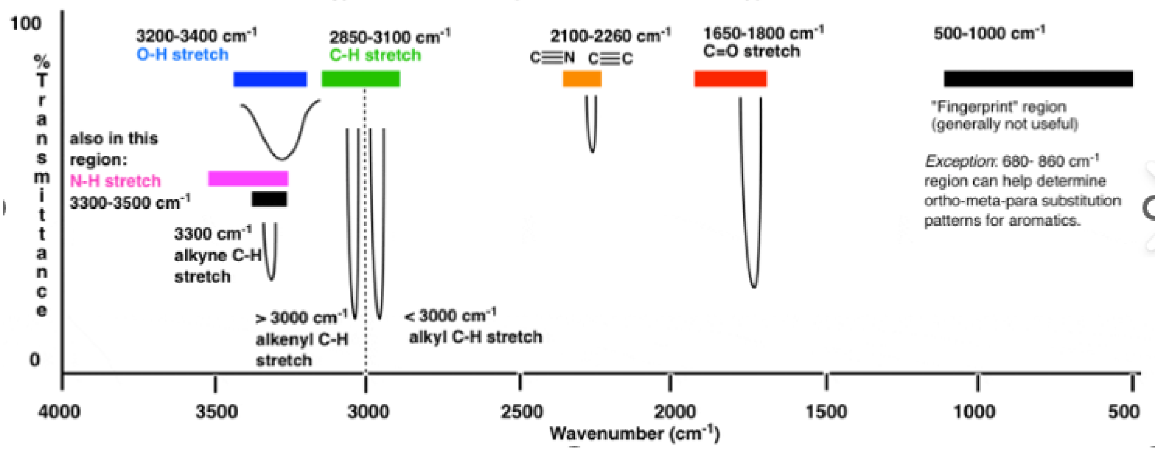


Figure 1-1 Typical infrared absorption values for various types of bonds

II. TYPES OF BONDS

Absorption of infrared radiation leads to changes in molecular oscillations in molecules and measurement of how bonds vibrate leads to infrared spectroscopy. Atom size, bond length, and bond strength vary in molecules, so the frequency at which a particular bond absorbs infrared radiation varies across a range of bonds and vibration states [12].

An organic molecule can have a whole range of different bonds. All these links will vibrate, and obviously different links will vibrate at different frequencies [4]. There are two basic modes of vibration which is as follows:

1. *Stretching*

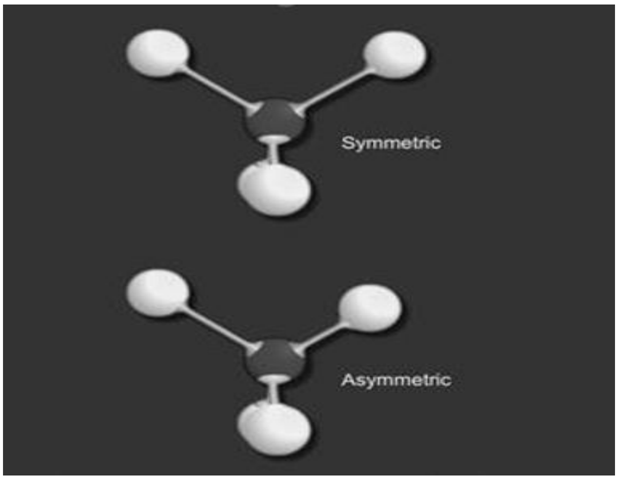


Figure 1-2 vibration in stretching mode

2. *Bending*

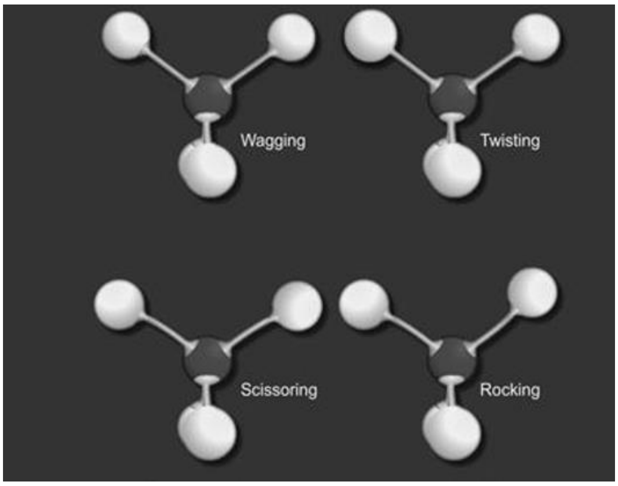


Figure 1-3 vibration in Bending mode

For a given covalent bond in the molecule, only a certain set of vibrational frequencies is possible [7]. Suppose that the link oscillates at frequencies v1 and its next available frequency is v2; then, when radiation with a frequency of (v2-v1) hits the compound containing this bond, some of the radiation is absorbed and the bond vibrates at a higher frequency [9].

ISSN: 2583-4053
Volume-2 Issue-5 || October 2023 || PP. 128-131
https://doi.org/10.55544/jrasb.2.5.21

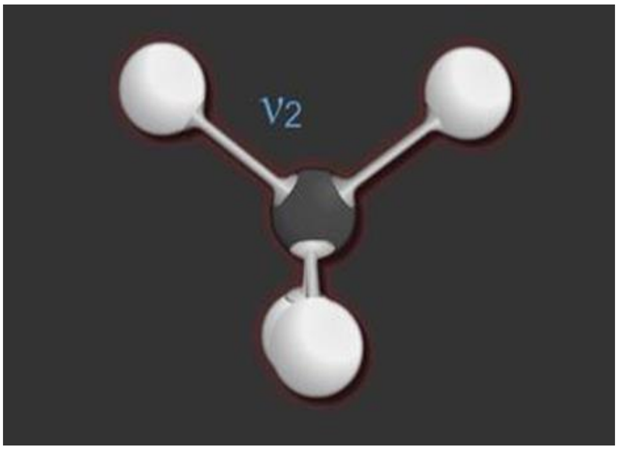


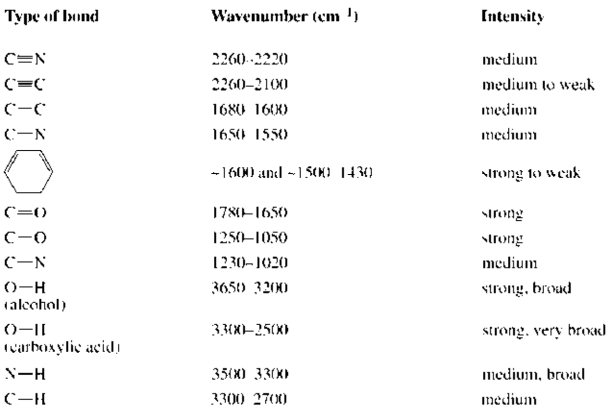
Figure 1-4 vibrational frequency in covalent Bond

The frequency for a given connection is independent of the other connection, thus, the determination of the frequency in the infrared range that are absorbed by the compound provides information about the types of bonds present [4].

An infrared spectrum analyzes a compound by passing infrared radiation through a sample in a range of different frequencies and measuring the absorption generated by each type of bond in the compound. The result is a spectrum, which is usually a graph of the transmittance ration versus the wavenumber [8].

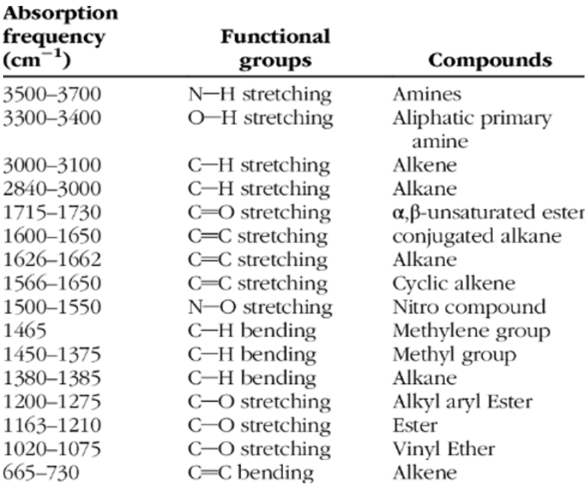
Since there are no two organic compounds with the same infrared spectrum, individual pure compounds can be identified by examining their spectra. In the range of 7-11 µm. there are many absorption bands and even pairs of almost identical organic molecules show difference here [5]. This region is called the fingerprint region and as long as the chemist has a copy of the spectrum, any unknown pure compound can be replaced [3].

The area, 2.5 -7 microns, is simpler and has lower absorption ranges. This area is used to identify structures, as certain groups can be identified more easily. Bending frequencies tend to be numerous, quite complex, and not much used for identification [11].



Type of bond	Wavenumber (cm $^{-1}$)	Intensity
C≡N	2260–2220	medium
C≡C	2260–2100	medium to weak
C—C	1680–1600	medium
C—N	1650–1550	medium
	~1600 and ~1500–1430	strong to weak
C=O	1780–1650	strong
C—O	1250–1050	strong
C—N	1230–1020	medium
O—H (alcohol)	3650–3200	strong, broad
O—H (carboxylic acid)	3300–2500	strong, very broad
N—H	3500–3300	medium, broad
C—H	3300–2700	medium

Figure 1.5 wavenumber and intensity of bonds in some organic compounds



Absorption frequency (cm $^{-1}$)	Functional groups	Compounds
3500–3700	N—H stretching	Amines
3300–3400	O—H stretching	Aliphatic primary amine
3000–3100	C—H stretching	Alkene
2840–3000	C—H stretching	Alkane
1715–1730	C=O stretching	α,β-unsaturated ester
1600–1650	C=C stretching	conjugated alkane
1626–1662	C=C stretching	Alkane
1566–1650	C=C stretching	Cyclic alkene
1500–1550	N—O stretching	Nitro compound
1465	C—H bending	Methylene group
1450–1375	C—H bending	Methyl group
1380–1385	C—H bending	Alkane
1200–1275	C—O stretching	Alkyl aryl Ester
1163–1210	C—O stretching	Ester
1020–1075	C—O stretching	Vinyl Ether
665–730	C=C bending	Alkene

Figure 1.6 Absorption frequency of bonds in organic compounds functional groups.

III. ANALYSES OF CHEMICAL BONDS IN HYDROCARBONS

a. Alkanes show very few absorption bands in the infrared spectrum. They yield four more C-H stretching peaks near 3000 cm^{-1} plus CH2 and CH3 bending peaks in the range 1475-1365 cm^{-1}. The spectrum is usually simple with few peaks. In alkanes (except strained ring compounds) sp^3 C-H absorption always occurs at frequencies less than 3000 cm^{-1} [5].

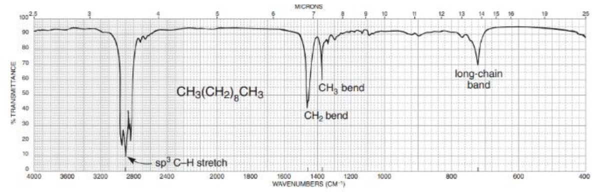


Figure 1-7 the infrared spectrum of decane

b. Alkenes show many more peaks than alkanes. The principles peaks of diagnostic value are the C-H stretching peaks for the sp^2 carbon at values greater that 3000cm^{-1}, along with C-H peaks for the sp^3 carbon atoms appearing below that value. Also prominent are the out of plan bending peaks that appear in the range 1000-650 cm^{-1}. For unsymmetrical compounds, you should expect to see the C=C stretching peak near 1650 cm^{-1}.

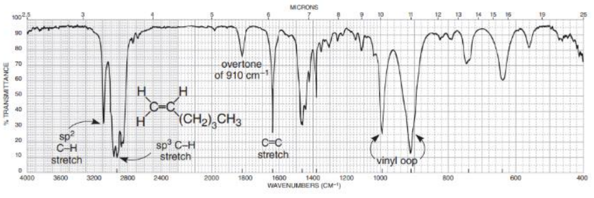


Figure 1-8 the infrared spectrum of hexene

c. Alkynes will show a prominent peak at about 3300 cm^{-1} for the sp-hybridized C-H. A carbon-to-carbon triple bond will also be a prominent feature in the spectrum for

ISSN: 2583-4053
Volume-2 Issue-5 || October 2023 || PP. 128-131

https://doi.org/10.55544/jrasb.2.5.21

the terminal alkyne, appearing at about 2150 cm^{-1}. The alkyl chain will show C-H stretching frequencies for the SP^3 carbon atoms. Other features include the bending bands for CH2 and CH3 groups. Nonterminal alkynes will not show the C-H band at 3300 cm^{-1} will be very weak or absent from the spectrum [6].

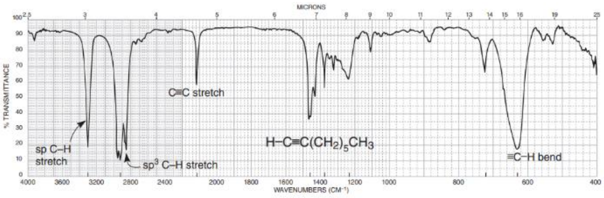


Figure 1-9 the infrared spectrum of 1-octyne

IV. CONCLUSION

By doing this research It is concluded that when analyzing the infrared spectrum in organic compounds, we must concentrate first efforts on determining the presence or absence of a few major functional group. The C=O, O-H, N-H, C-O, C=C and NO2 peaks are the most conspicuous and give immediate structural information if they are present. We do not have to try to make a detailed analysis of the C-H absorption near 3000cm-1 almost all the compounds have this absorption. No need to worry about subtilities of the exact environment in which the functional group is found.

REFERENCES

[1] Bellamy, L. J., The Infrared Spectra of Complex Molecules, 3rd ed., John Wiley, New York, 1975

[2] Colthrup, N. B., L. H. Daly, and S. E. Wiberley, Introduction to Infrared and Raman Spectroscopy, 3rd ed., Academic Press, New York, 1990

[3] Lin-Vien, D., N. B. Colthrup, W. G. Fateley, and J. G. Grasselli, The Handbook of Infrared and Raman Characteristic Frequencies of Organic Molecules, Academic Press, New York, 1991.

[4] Nakanishi, K., and P. H. Solomon, Infrared Absorption Spectroscopy, 2nd ed., Holden–Day, San Francisco, 1998. Pouchert, C. J., Aldrich Library of FT-IR Spectra, Aldrich Chemical Co., Milwaukee, WI, 1985 (1st ed.) and 1997 (2nd ed.).

[5] Pretsch, E., T. Clerc, J. Seibl, and W. Simon, Tables of Spectral Data for Structure Determination of Organic Compounds, 3rd ed., Springer-Verlag, Berlin, 1998, 1989. Translated from the German by K. Biemann

[6] Pretsch, E., T. P. Buhlmann, and C. Affolter, Structure Determination of Organic Compounds. Tables of Spectral Data, 4th ed., Springer-Verlag, Berlin and New York, 2009.Silverstein, R. M., F. X. Webster, and D. Kiemle, Spectrometric Identification of Organic Compounds, 7th ed., John Wiley, New York, 2005

[7] Chapman, J. R., Practical Organic Mass Spectrometry: A Guide for Chemical and Biochemical Analysis, 2nd ed., John Wiley, New York, 1995.

[8] Gross, J. H., and Roepstorff, Mass Spectrometry: A Textbook, 2nd ed., Springer, Berlin, 2011.

[9] Lambert, J. B., S. Gronert, H. F. Shurvell, and D. A. Lightner, Organic Structural Spectroscopy, 2nd ed., Prentice Hall, Upper Saddle River, NJ, 2011.

[10] Pretsch, E., T. P. Buhlmann, and C. Affolter, Structure Determination of Organic Compounds. Tables of Spectral Data, 4th ed., Springer-Verlag, Berlin and New York, 2009

[11] Watson, J. T. and O. D. Sparkman, Introduction to Mass Spectrometry: Instrumentation, Applications, and Strategies for Data Interpretation, 4th ed., Wiley, New York, 2007.