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# Vibrational Spectra of Organic Compounds

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**ABSTRACT:** The increasing demand for product quality improvement and production rationalization in the chemical, petrochemical, polymer, pharmaceutical, cosmetic, food, and agricultural industries has induced a significant renaissance of the vibrational spectroscopic techniques of Raman, infrared (IR), and near-infrared (NIR) spectroscopy. This trend has partly led to the gradual substitution of time consuming conservative analytical techniques (gas chromatography (GC), high-performance liquid chromatography (HPLC), nuclear magnetic resonance (NMR), and mass spectroscopy (MS)) and nonspecific control procedures (temperature, pressure, pH, and dosing weight) by the more specific and environmentally compatible analytical tools of vibrational spectroscopy. Thus, infrared (IR), NIR, and Raman spectroscopy have emerged over the last decade – in combination with imaging accessories, light-fiber optics, new in-line and on-line probes, and chemometric evaluation procedures – as extremely powerful methods for industrial research, quality control, and process monitoring. Specifically, the NIR wavelength gap between the visible and the IR region, which has over a long period been lying idle, has eventually also been filled with life and is now used according to its real potential.

Synthetic polymers have become an integral part of our everyday life and this article will demonstrate that the vibrational spectroscopic techniques are extremely important characterization and control tools for the whole life cycle of a polymeric product. Although some theoretical, instrumental, and experimental background of vibrational spectroscopy will be provided, the ultimate source for a complete coverage of these topics is certainly the Handbook of Vibrational Spectroscopy and a more recent polymer-dedicated offspring.<sup>1,2</sup> The principal aim of this article is to demonstrate to the reader with the help of selected examples the broad range of applicability of the three techniques and encourage him to fully exploit their potential for the characterization of the chemical and physical properties of polymers. The main focus is the comparative treatment of the three vibrational spectroscopic techniques in such a manner that the reader can form his opinion on the pros and cons for the discussed applications and transfer these conclusions to his own field of activity. The technique of far-infrared (FIR) spectroscopy,<sup>3,4</sup> which is now better known and mainly operated as terahertz (THz) spectroscopy,<sup>5</sup> is much less frequently used for the characterization of polymers and will, therefore, be discussed only briefly. It has to be emphasized, however, that despite the uncontested importance of the vibrational spectroscopies for the characterization of macromolecular structure, only a limited number of problems may be solved by the exclusive application of these techniques. Thus, in the majority of analytical investigations of polymer constitution and any additives, chemical separation of the components is inevitable; a more complete picture of the sequence distribution and stereoregularity of structural units in polymers is obtained only in combination with NMR spectroscopy; the results of vibrational spectroscopic investigations of polymers at elevated temperatures are advantageously correlated with differential scanning calorimetry (DSC) and last but not least, a thorough knowledge of the structure of crystalline polymers cannot be attained without application of X-ray diffraction. These few, far from comprehensive, examples demonstrate that maximum information on the structural details in question can be obtained only by an appropriate choice and combination of chemical and physical methods.

**KEYWORDS:** vibration, organic, compounds, spectra, polymers, chromatography, diffraction, IR, X-ray

## I. INTRODUCTION

Vibrational spectroscopy is concerned with the transitions due to absorption or emission of electromagnetic radiation. These transitions appear in the range of  $10^2$  to  $10^4$   $\text{cm}^{-1}$  and originate from the vibration of nuclei constituting the molecules. A chemical bond in a molecule can vibrate in many ways, and each vibration is called vibrational mode. There are two types of molecular vibrations, stretching and bending. A stretching vibration is characterized by movement along the bond axis [1,2] with increasing or decreasing of the interatomic distances, whereas a bending vibration consists of a change in bond angles with respect to the remainder of the molecule. The two widely used spectroscopic techniques based on vibrational energy are the Raman spectroscopy and the infrared spectroscopy. Both



methods give complementary information and are based on the fact that within any molecules the atoms vibrate with a few definite sharply defined frequency characteristics of that molecule. When a sample is irradiated to a beam of incident radiation, it absorbs energy at frequencies characteristic to that of the frequency of the vibration of chemical bonds present in the molecules. This absorption of energy by vibrating chemical bond results in an Infrared spectrum. Raman spectroscopy is a scattering phenomenon, and arises due to the difference between the incident and scattered radiation frequencies. It utilizes scattered light to gain knowledge about molecular vibration, which can provide information regarding the structure, symmetry, electronic environment, and bonding of the molecule.[3,4]

Vibrational spectroscopy had been widely used in both academia and industry as an important tool in the structural characterization of compounds and analysis of impurities. In particular infrared spectroscopy in this field shows remarkable progress. One of the great advantages of Fourier transform infrared (FTIR) for natural products analysis over other techniques is that spectra can be obtained from almost any environment and from relatively small quantities of samples. Moreover, infrared (IR) techniques, when coupled with intensity measurement, may be used both for qualitative and quantitative analysis [1]. With the introduction of FTIR spectrometers and lasers as the source for recording the Raman spectra, vibrational spectroscopy has become an effective tool for the elucidation of molecular structure. IR spectroscopic techniques such as ATR[5,6] (attenuated total reflectance) provide convenient measurement of most liquid samples such as edible oil and plant extract in routine use. Thus, there is no excessive sample preparation, so the use of hazardous solvents and reagents can be avoided [2]. For this reason, FTIR spectroscopy and other vibrational spectroscopic techniques can be taken into consideration as a “green analytical technique” for the analysis of edible fats and oils [3]. Discovery of FTIR and Raman spectroscopy techniques with recent innovations in Raman spectroscopy with laser as the source of light[7,8] and the availability of a fluorescence free Raman spectra has renaissance the application of vibrational spectroscopy in various fields at a remarkable level [4].

Vibrational spectroscopy has advantages over the widely used NMR spectroscopy techniques in many aspects such as short analysis time, less quantity requirement, and the possibility for situ analysis of biological samples and nondestructive analysis mode. Although it gives less information on the exact chemical structure of the molecule, this technique is an indispensable and widely used fast analytical process and can be used as a fingerprint for identification and comparison of compounds [5], which allows this method to be used not only in structure characterization but also in other fields such as quality control in food industries [6] and forensic sciences [7]. In subsequent sections of the chapter, we will review the basic principles of vibrational spectroscopy and their applications in the structure characterization of compounds, particularly with reference to the biologically significant compounds.[9,10]

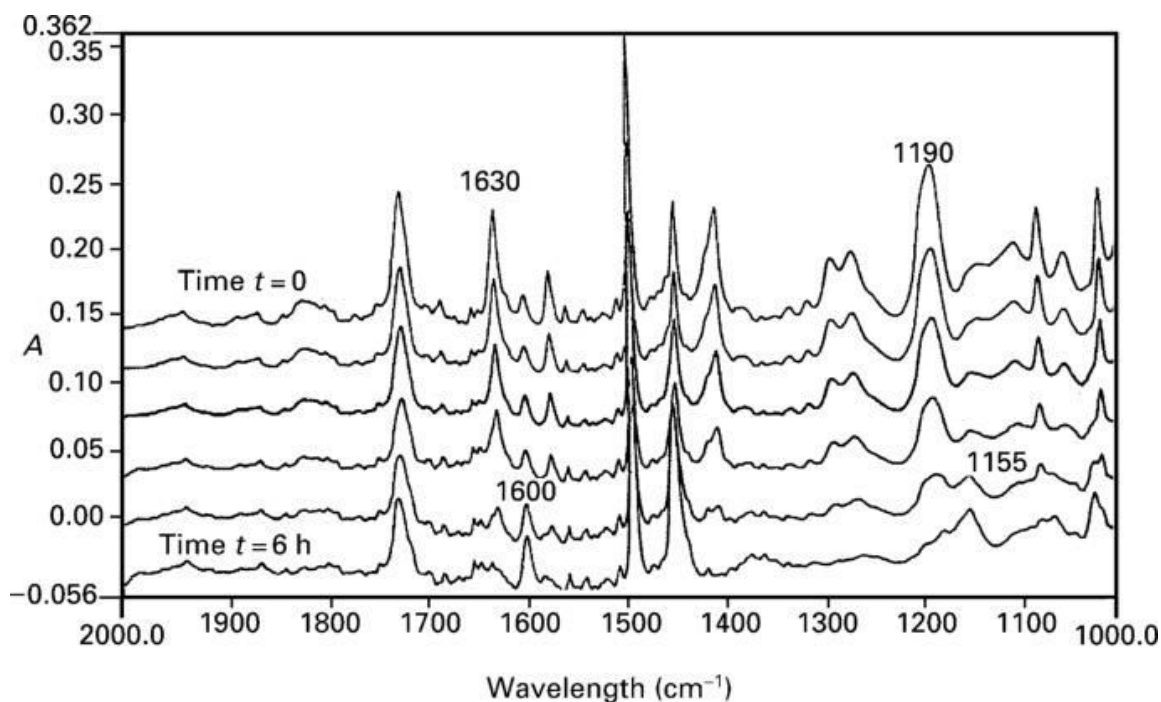
Vibrational spectroscopy is a technique that results from the vibrational motions of molecules and can be used to determine molecular structure and to report on local environments, including solvation effects, ion pairing, intermolecular interaction strengths, and ion–molecule binding, to name a few applications. Molecular vibrations are highly sensitive to environment, intermolecular forces, temperature, and local electric fields exerted by adjacent ions. One can theoretically use vibrational spectroscopy to identify molecules in complex mixtures. However, a second complementary experimental method is most often needed in such highly complex mixtures. [11,12] Nevertheless, molecular moieties such as nitrates and sulfates present highly distinctive vibrations and can be identified using vibrational spectroscopic methods. Because molecular vibrational spectral features are so highly sensitive to environment and to adjacent atoms and their arrangements within the molecule, their spectrally observed frequencies and intensities can vary, sometimes by more than 100 cm<sup>-1</sup>. To this point, in an aqueous solution, this sensitivity to local environment can simplify assignment of specific molecular vibrations within the spectrum. In two- or three-component gas and liquid mixtures, identification of compounds having low atomic complexity can be easily ascertained, and this is commonly done for laboratory kinetic and reaction rate constant measurements.[13,14]

Interestingly, the sensitivity of molecular vibrations to intra- and intermolecular forces provides a versatile means to interpret organization of the molecule in its local environment. Frequency shifts reveal strengthening or weakening of the bond (i.e., the energies of molecular orbitals). Intensity changes reveal the bond response of the molecule to the incident electric field and are denoted as the transition moment strength. The combination of frequency shifting with intensity changes sometimes presents great challenges to deconvolute these contributions to the spectrum. Thus, theoretical support is quite often an important aspect of deciphering complexities of the spectrum itself. This provides a great collaborative opportunity for both the experimentalist and theorist. Yet, through a methodical series of control experiments, it is quite often possible to delineate spectral features to then provide decisive information about the molecular organization and local environment.[15,16]

Vibrational spectroscopy experimental techniques are not generally touted for their low detection limits, typically in the mM range. However, surface-selective methods can detect even submonolayer coverage of surfaces, and many times with ease due to the inherent capabilities of certain spectroscopic techniques, particularly nonlinear spectroscopic methods such as sum-frequency generation (SFG).<sup>6</sup> In addition, surface enhancement on electron-rich solids can be attained by use of surface plasmon enhancement techniques, for example, the use of metallic thin films/structures in surface-enhanced Raman spectroscopy.<sup>[17,18]</sup>

Vibrational spectroscopy continues to be an important tool for qualitative and quantitative measurements, for example, to assess intermediates in chemical reactions of aqueous phases, to understand solvation and ion pairing, and to monitor reaction kinetics. With respect to atmospherically related systems, water as the solvent medium and hydration at interfaces have been studied extensively. Vibrational spectroscopy is an important tool being utilized increasingly in the field where robust field-tested Raman and infrared (IR) instruments are commonly used to identify chemical speciation and intermolecular interactions in laboratory studies. Additionally, laboratory studies of field-collected samples have been explored.<sup>7</sup> This chapter focuses on interfacial spectroscopic methods and the application of both IR and spontaneous Raman for interrogation of interfaces, specifically in the context of aqueous surfaces.<sup>[19,20]</sup>

Vibrational spectroscopy is a valuable tool for the elucidation of molecular structure. The transitions between vibrational states of a molecule are observed experimentally via infrared and Raman spectroscopy. These techniques can be used to determine a molecule's structure and environment since these factors affect the vibrational frequencies.<sup>[21,22]</sup>



**Fig. In situ infrared spectra measured during the progress of a copolymerization reaction using a fibreoptic probe.**

Vibrational spectroscopy provides important information about the nature of chemical bond, intramolecular forces acting between the atoms in a molecule, and intermolecular forces in condensed phase. In order to gain such useful information, it is necessary to assign vibrational motion corresponding to each peak in the spectrum. This assignment can be quite difficult due to the large number of closely spaced peaks even in fairly simple molecules. In order to aid in this assignment, computer simulations are used to calculate the vibrational frequencies of molecules. Ever since Pulay and collaborators popularized the calculation of molecular force fields in the 1970s, there has been considerable<sup>[23,24]</sup> interest among theoretical chemists to determine ever more accurate force fields for the prediction of rotational–vibrational spectra, the evaluation of vibrationally averaged properties and thermodynamic functions, the determination of many-body potentials, and for other purposes. As for the prediction of vibrational spectra of large molecules, the use



of HF ab initio or DFT methods for determining whole or partial force fields has also benefitted greatly from the advances made in quantum chemical methodology. The rapidly growing impact that computational studies are having in this important area of research is amply demonstrated by the different types of systems under investigation, ranging from small molecules to polymeric systems and liquid crystals.[25,26]

## II. DISCUSSION

Raman spectroscopy in conjunction with infra red spectroscopy and other physical techniques such as D.S.C and X-ray diffraction has been used to study the structure of organic compounds and polymers. Characteristic Raman frequencies have been deduced for a variety of molecular backbones and groups belonging to substituted benzenes. These have been shown to be particularly useful where polar substituents such as carbonyl and nitro groups are involved. Nevertheless, the joint use of Raman and IR frequencies usually provides much more information than either Raman or IR. Considerable expertise has been developed in the synthesis of a large number of polymers and their subsequent handling and processing.[27,28] The observation of correlation band splitting and longitudinal acoustic modes which occur at very low frequencies in the Raman spectrum have been particularly emphasised because of their significance to the interpretation of polymer structure. Conclusions reached from the analysis of vibrational spectra of polyethers and polythioethers of the frequencies  $f(\text{CH}_2) - l_j$  ( $m = 1-6, 10$ ;  $Y = 0$  or  $S$ ), may be summarised as follows: M nA careful analysis of the molecular vibrations of these polymers has been carried out before looking for correlation band splitting in their spectra. Assignments for the observed bands have been made on the basis of reported calculations or on tentative basis. Correlation band splitting has been observed in the spectra of polyethylene oxide, polydecamethylene oxide and polythioethers with  $m = 2-6$  and  $10$ .[29,30] It has been shown, however, that its occurrence in the spectra of polydecamethylene oxide and polythioethers with  $m > 4$  is dependent upon the mode of crystallization and annealing. These observations have been applied to deduce molecular and crystal structures of these polymers. The longitudinal acoustic modes observed at very low frequencies in the Raman spectra of polyethers with  $m = 4, 6$  and  $10$  and polythioethers (with  $m = 2-6$  and  $10$ ) indicate that the crystallization of these polymers is predominantly lamellar. Crystallization from solution result in very thin lamellae which thicken on annealing just below  $T_M^*$  Melt crystallization, however, gives rise to well developed lamellae which thicken further on annealing. Although the application of Raman technique to this field is limited because of experimental difficulties, it offers a number of advantages over other techniques such as low angle X-ray diffraction electron microscopy etc. It is concluded that Raman spectroscopy is a powerful analytical technique which when applied in conjunction with other techniques, yields very much valuable information about the structure of organic compounds and polymers.[31]

Until the mid-20th century, most organic compounds were distinguished from one another largely on the basis of simple physical and chemical properties. Knowledge of these properties, however, yields only superficial clues about a compound's molecular structure, and the determination of that structure was a complicated process (for large molecules at least) that involved careful analysis of several reaction pathways. Chemists had no way to see what molecules looked like, because molecules are so small that no device such as a microscope could be developed that would give a complete image of a molecular structure. One technique, X-ray crystallography, can give precise structural data for some molecules, but only those that can be obtained in solid, crystalline form. Normally, a full X-ray structure determination is a costly, time-consuming endeavour that is applied to only the most puzzling structures. Sufficient information to decipher a molecule's structure is much more easily obtained by the use of one or more spectroscopic techniques.[32]

Spectroscopy is a general term used for the instrumental processes by which information about molecular structure is obtained through careful analysis of the absorption, scattering, or emission of electromagnetic radiation by compounds. Electromagnetic radiation is the continuous spectrum of energy-bearing waves ranging from extremely short waves, such as high-energy X-rays (with wavelengths of about 10 nanometres [nm]), to very long, low-energy waves such as radio waves (with wavelengths of one metre [m] or more). Visible light, for example, is the range of electromagnetic radiation detectable by human vision, with wavelengths of roughly 400 to 700 nm. Objects appear coloured when they absorb visible light of certain wavelengths, and those absorbed wavelengths are consequently absent from light that passes from the coloured object to the eyes.[33]

Molecules are able to absorb light of certain wavelengths because the energy content of the absorbed light is the precise value needed to cause a molecule to be excited from one energy state to a higher one. The myriad energy levels in a molecule are said to be quantized because each one differs from another by a discrete, measurable energy value, just as each step in a stairway is a fixed height above, or below, all others. Thus, by measuring the wavelengths of the

electromagnetic radiation absorbed by a molecule, it is possible to gain information about the various energy levels within it. This information can then be correlated with specific details of molecular structure. Instruments called spectrometers measure the wavelengths of light that are absorbed by molecules in various regions of the electromagnetic spectrum. The most important spectroscopic techniques for structure determination are ultraviolet and visible spectroscopy, infrared spectroscopy, and nuclear magnetic resonance spectroscopy. A fourth technique, termed mass spectrometry, does not depend on absorption of electromagnetic radiation, but it is valuable for the information it provides about the number and type of atoms present in a molecule.[34,35]

Most organic compounds are transparent to the relatively high-energy radiation that constitutes the ultraviolet (200–400 nm) and visible (400–700 nm) portion of the electromagnetic spectrum, and consequently they appear colourless in solution. This is because the electrons in the  $\sigma$  bonds of organic molecules require wavelengths of even higher energy (such as those of X-rays) to excite them to the next higher accessible energy level. Electrons in  $\pi$  bonds, however, can be promoted to higher energy levels by ultraviolet and visible light, and UV-visible spectroscopy consequently provides useful structural information for molecules that contain  $\pi$  bonds. When multiple  $\pi$  bonds are separated from each other by intervening single bonds, they are said to be conjugated. The UV-visible spectrum of a molecule is dramatically affected by the presence of conjugation. As the number of conjugated  $\pi$  bonds increases, the UV-visible spectrum shows light absorption at a greater number of different wavelengths (i.e., the spectrum contains more absorption peaks), and light of longer wavelengths (and lower energy) is absorbed. The many individual peaks of UV-visible spectra normally coalesce to produce a continuous absorption spectrum, with some of the strongest individual absorption peaks appearing as sharp spikes. For example, the UV-visible spectrum of azulene, a molecule that contains five conjugated  $\pi$  bonds, shows a strong absorbance in the visible region of the electromagnetic spectrum, which correlates with its intense blue colour.[36,37]

Naturally occurring organic compounds that are highly coloured contain an extensive system of conjugated  $\pi$  bonds. The compound largely responsible for the bright orange colour of carrots,  $\beta$ -carotene, contains 11 conjugated  $\pi$  bonds. UV-visible spectroscopy is especially informative for molecules that contain conjugated  $\pi$  bonds. In organic compounds, atoms are said to be bonded to each other through a  $\sigma$  bond when the two bonded atoms are held together by mutual attraction for the shared electron pair that lies between them. The two atoms do not remain static at a fixed distance from one another, however. They are free to vibrate back and forth about an average separation distance known as the average bond length. These movements are termed stretching vibrations. In addition, the bond axis (defined as the line directly joining two bonded atoms) of one bond may rock back and forth within the plane it shares with another bond or bend back and forth outside that plane. These movements are called bending vibrations. Both stretching and bending vibrations represent different energy levels of a molecule. These energy differences match the energies of wavelengths in the infrared region of the electromagnetic spectrum—i.e., those ranging from 2.5 to 15 micrometres ( $\mu\text{m}$ ;  $1 \mu\text{m} = 10^{-6} \text{m}$ ). An infrared spectrophotometer is an instrument that passes infrared light through an organic molecule and produces a spectrum that contains a plot of the amount of light transmitted on the vertical axis against the wavelength of infrared radiation on the horizontal axis. In infrared spectra the absorption peaks point downward because the vertical axis is the percent transmittance of the radiation through the sample. Absorption of radiation lowers the percent transmittance value. Since all bonds in an organic molecule interact with infrared radiation, IR spectra provide a great deal of structural data.[38,39]

### III. RESULTS

The stretching vibrations of strong carbon-hydrogen bonds cause the absorptions around  $3.4 \mu\text{m}$ , with the sharp peak at  $3.2 \mu\text{m}$  due to the hydrogen atom on the carbon-carbon double bond. The many bending vibrations of carbon-hydrogen bonds cause the complicated absorption pattern ranging from about 7 to  $25 \mu\text{m}$ . This area of IR spectra is called the fingerprint region, because the absorption pattern is highly complex but unique to each organic structure. The stretching vibrations for both the carbon-carbon and carbon-oxygen double bonds are easily identified at  $6.1 \mu\text{m}$  and  $5.8 \mu\text{m}$ , respectively. Most of the functional groups have characteristic IR absorptions similar to those for carbon-oxygen and carbon-carbon double bonds. Infrared spectroscopy is therefore extremely useful for determining the types of functional groups present in organic molecules.

Absorption of long-wavelength (1–5 m) low-energy radiation in the radio-frequency region of the electromagnetic spectrum is due to the atomic nuclei in a molecule. Many (but not all) atomic nuclei have a small magnetic field, which makes them behave somewhat like tiny bar magnets. When placed in a strong external magnetic field, such nuclei can assume different energy states; in the simplest case, two energy states are possible. In the lower energy state, the magnetic field of the nucleus is aligned with the external magnetic field, and, in the higher energy state, it is aligned

against the field. The energy difference between the two levels depends on the strength of the external magnetic field. In modern NMR spectrometers, organic compounds are placed in magnetic fields ranging from about 1.4 to 18.0 teslas (T) and are irradiated with radio-frequency waves. For comparison,[40,41] the Earth's magnetic field is about 0.00007 T. At a magnetic-field strength of 1.4 T, the energy difference between the lower and higher energy states of a  $^1\text{H}$  proton nucleus is only 0.024 J mol<sup>-1</sup>. Electromagnetic radiation with a frequency of about 60 megahertz (MHz) can supply the energy needed to convert the lower energy state to the higher one. The energy difference between the magnetic energy levels of a nucleus is measured as an absorption peak, or a resonance. Because the energy of the absorbed radiation depends on the environment around the absorbing nucleus in a molecule, NMR spectroscopy provides the most structural information of all the spectroscopic techniques used in chemistry. Especially valuable are proton magnetic resonance spectroscopy, which measures the resonances due to energy absorption by hydrogen atoms in organic compounds, and carbon-13 magnetic resonance spectroscopy, which yields the resonances due to absorption by atoms of carbon-13 ( $^{13}\text{C}$ ), a naturally occurring isotope of carbon that contains six protons and seven neutrons.

Proton NMR spectra yield a great deal of information about molecular structure because most organic molecules contain many hydrogen atoms, and the hydrogen atoms absorb energy of different wavelengths depending on their bonding environment.[41]

NMR absorbances appear in a spectrum as a series of sharp spikes or peaks. Although there is no vertical scale on the spectrum, the relative height of each peak corresponds roughly to the strength of the absorption. The horizontal scale does not show proton resonances in simple wavelength units. Instead, the position of each peak is normally measured relative to the absorption of the protons in the compound tetramethylsilane,  $(\text{CH}_3)_4\text{Si}$ . Tetramethylsilane is an inert liquid added in small amounts to the compound being analyzed. All 12 of its hydrogen atoms absorb at the same position to give a single sharp peak, which is arbitrarily assigned a positional value of zero. This peak is then used as a reference point for all other peaks in the spectrum. The hydrogen atoms in the molecule being analyzed generally appear to the left of the reference peak because they absorb radiation of higher energy than the hydrogens of tetramethylsilane.

The distance of the proton absorptions from the reference peak is given by a number called the chemical shift. Each unit of chemical shift represents a fractional increase of one part per million (ppm) in the energy of absorbed radiation, relative to the value for tetramethylsilane. For example, in the proton NMR spectrum of bromoethane, the hydrogen atoms of the  $\text{CH}_3$  group appear at about 1.6 ppm and the hydrogens of the  $\text{CH}_2$  group at about 3.3 ppm. Atoms in a molecule have different chemical shifts because they experience slightly different local magnetic fields owing to the presence of nearby electrons. Electrons generate a magnetic field of their own, which reduces the magnitude of the total field at the nucleus. Nuclei that are surrounded by regions of high electron density, such as the hydrogen atoms of tetramethylsilane, are said to be shielded from the applied field of the instrument's magnet. The electronegative bromine atom in bromoethane pulls electrons away from the carbon and hydrogen atoms. The  $\text{CH}_2$  hydrogens are more strongly affected than the  $\text{CH}_3$  hydrogens and thus have a greater chemical shift, because they are closer to the bromine atom. All three hydrogens on the  $\text{CH}_3$  group are exposed to the same local magnetic field and consequently have the same chemical shift. Such hydrogens are said to be equivalent. The two hydrogens on the  $\text{CH}_2$  group are also equivalent. The chemical shift of hydrogen atoms is the most important piece of information provided by NMR spectroscopy, because it reveals a great deal about the nature of the bonds around the hydrogen.[38]

Two more features of NMR spectra are important aids to structure assignment. The first is the area of space enclosed by the absorption peaks. The area under the peaks is directly proportional to the number of hydrogen atoms contributing to the peak. NMR spectrometers have a feature, called integration, which, when selected by the user, calculates the area under each peak and plots the result as a line that is displaced vertically at a peak by an amount proportional to the area under the peak. The integration of the bromoethane spectrum, for example, shows that the absorption peaks around 1.6 ppm have an area that is 1.5 times greater than the area of the peaks at 3.3 ppm. This is consistent with, and supports, the assignment of the peaks to the  $\text{CH}_3$  and  $\text{CH}_2$  groups because the ratio of the area of the  $\text{CH}_3$  peak to the  $\text{CH}_2$  peak is expected to be 3:2, or 1.5:1, for the numbers of hydrogen atoms are in a 3:2 ratio.

The second additional feature is the pattern of the absorption peaks. In the bromoethane example, the  $\text{CH}_3$  peak is split into three distinct peaks, called a triplet. The  $\text{CH}_2$  peak is split into four peaks, called a quartet. These multiple peaks are caused by nearby hydrogen atoms through a process termed spin-spin splitting. Each set of equivalent hydrogens on a given carbon is split into an  $n+1$  multiplet by adjacent hydrogen atoms that are nonequivalent to the hydrogens of the



given carbon. These splittings are generally observed for all nonequivalent hydrogens bonded to the one or two adjoining carbon atoms. In the bromoethane spectrum, the  $\text{CH}_3$  absorption appears as a triplet owing to the effects of the two hydrogens on the adjacent  $\text{CH}_2$  group. Reciprocally, the  $\text{CH}_2$  absorption is a quartet because of the effects of the three hydrogen atoms on the neighbouring  $\text{CH}_3$  group.[37]

#### IV. CONCLUSIONS

To calculate vibrational spectra of organic molecules

The usual approach is:

- Find the equilibrium geometry (within the Born-Oppenheimer app.).
- Expand the energy in Taylor series till second order term. The first order will be 0 because of the minimum energy condition.
- Include this expression in the Hamiltonian.
- Generate a coordinate transformation to get normal coordinates.
- Relate second order derivative of the potential energy with the force constant of Hook law (Using second order term we can identify it with a harmonic oscillator). Then get the harmonic frequencies.
- The software employed should give also the intensity for each frequency.
- Plot intensity vs. frequency/energy/wave length. You'll get only "points". To transform them to a continuous function you can use a Lorentzian like function.[42]

#### REFERENCES

1. Zeitler JA, Taday PF, Newnham DA, Pepper M, Gordon KC, Rades T (February 2007). "Terahertz pulsed spectroscopy and imaging in the pharmaceutical setting--a review". *The Journal of Pharmacy and Pharmacology*. 59 (2): 209–23. doi:10.1211/jpp.59.2.0008. PMID 17270075. S2CID 34705104.
2. ^ Atkins PW, de Paula J (2009). *Elements of physical chemistry* (5th ed.). Oxford: Oxford U.P. p. 459. ISBN 978-0-19-922672-6.
3. ^ Schrader B (1995). *Infrared and Raman Spectroscopy: Methods and Applications*. New York: VCH, Weinheim. p. 787. ISBN 978-3-527-26446-9.
4. ^ Harwood LM, Moody CJ (1989). *Experimental organic chemistry: Principles and Practice* (Illustrated ed.). Wiley-Blackwell. p. 292. ISBN 978-0-632-02017-1.
5. ^ Shadman S, Rose C, Yalin AP (2016). "Open-path cavity ring-down spectroscopy sensor for atmospheric ammonia". *Applied Physics B*. 122 (7): 194. Bibcode:2016ApPhB.122..194S. doi:10.1007/s00340-016-6461-5. S2CID 123834102.
6. ^ Chromatography/Fourier transform infrared spectroscopy and its applications, by Robert White, p7
7. ^ H M Pollock and S G Kazarian, *Microspectroscopy in the Mid-Infrared*, in *Encyclopedia of Analytical Chemistry* (Robert A. Meyers, Ed, 1-26 (2014), John Wiley & Sons Ltd,
8. ^ Pollock Hubert M (2014). "Microspectroscopy in the Mid-Infrared". *Encyclopedia of Analytical Chemistry*. pp. 1–26. doi:10.1002/9780470027318.a5609.pub2. ISBN 9780470027318.
9. ^ H M Pollock and D A Smith, *The use of near-field probes for vibrational spectroscopy and photothermal imaging*, in *Handbook of vibrational spectroscopy*, J.M. Chalmers and P.R. Griffiths (eds), John Wiley & Sons Ltd, Vol. 2, pp. 1472 - 1492 (2002)
10. ^ Krivanek OL, Lovejoy TC, Dellby N, Aoki T, Carpenter RW, Rez P, et al. (October 2014). "Vibrational spectroscopy in the electron microscope". *Nature*. 514 (7521): 209–12. Bibcode:2014Natur.514..209K. doi:10.1038/nature13870. PMID 25297434. S2CID 4467249.
11. ^ Idrobo JC, Lupini AR, Feng T, Unocic RR, Walden FS, Gardiner DS, et al. (March 2018). "Temperature Measurement by a Nanoscale Electron Probe Using Energy Gain and Loss Spectroscopy". *Physical Review Letters*. 120 (9): 095901. Bibcode:2018PhRvL.120i5901I. doi:10.1103/PhysRevLett.120.095901. PMID 29547334.



12. ^ Lagos MJ, Batson PE (July 2018). "Thermometry with Subnanometer Resolution in the Electron Microscope Using the Principle of Detailed Balancing". *Nano Letters*. 18 (7): 4556–4563. Bibcode:2018NanoL..18.4556L. doi:10.1021/acs.nanolett.8b01791. PMID 29874456. S2CID 206748146.
13. ^ Hachtel JA, Huang J, Popovs I, Jansone-Popova S, Keum JK, Jakowski J, et al. (February 2019). "Identification of site-specific isotopic labels by vibrational spectroscopy in the electron microscope". *Science*. 363 (6426): 525–528. Bibcode:2019Sci...363..525H. doi:10.1126/science.aav5845. PMID 30705191.
14. ^ Hage FS, Nicholls RJ, Yates JR, McCulloch DG, Lovejoy TC, Dellby N, et al. (June 2018). "Nanoscale momentum-resolved vibrational spectroscopy". *Science Advances*. 4 (6): eaar7495. Bibcode:2018SciA...4.7495H. doi:10.1126/sciadv.aar7495. PMC 6018998. PMID 29951584.
15. ^ Senga R, Suenaga K, Barone P, Morishita S, Mauri F, Pichler T (September 2019). "Position and momentum mapping of vibrations in graphene nanostructures". *Nature*. 573 (7773): 247–250. arXiv:1812.08294. Bibcode:2019Natur.573..247S. doi:10.1038/s41586-019-1477-8. PMID 31406319. S2CID 118999071.
16. ^ Lagos MJ, Trügler A, Hohenester U, Batson PE (March 2017). "Mapping vibrational surface and bulk modes in a single nanocube". *Nature*. 543 (7646): 529–532. Bibcode:2017Natur.543..529L. doi:10.1038/nature21699. PMID 28332537. S2CID 4459728.
17. ^ Govyadinov AA, Konečná A, Chuvilín A, Vélez S, Dolado I, Nikitin AY, et al. (July 2017). "Probing low-energy hyperbolic polaritons in van der Waals crystals with an electron microscope". *Nature Communications*. 8 (1): 95. arXiv:1611.05371. Bibcode:2017NatCo...8...95G. doi:10.1038/s41467-017-00056-y. PMC 5522439. PMID 28733660.
18. ^ Venkatraman K, Levin BD, March K, Rez P, Crozier PA (2019). "Vibrational spectroscopy at atomic resolution with electron impact scattering". *Nature Physics*. 15 (12): 1237–1241. arXiv:1812.08895. Bibcode:2019NatPh..15.1237V. doi:10.1038/s41567-019-0675-5. S2CID 119452520.
19. ^ Henschel H, Andersson AT, Jaspers W, Mehdi Ghahremanpour M, van der Spoel D (May 2020). "Theoretical Infrared Spectra: Quantitative Similarity Measures and Force Fields". *Journal of Chemical Theory and Computation*. 16 (5): 3307–3315. doi:10.1021/acs.jctc.0c00126. PMC 7304875. PMID 32271575.
20. ^ Smith JG (2011). "Chapter 13 Mass Spectrometry and Infrared Spectroscopy". In Hodge T, Nemmers D, Klein J (eds.). *Organic chemistry* (3rd ed.). New York, NY: McGraw-Hill. pp. 463–488. ISBN 978-0-07-337562-5. Archived from the original (Book) on 2018-06-28. Retrieved 2018-06-30.
21. ^ Badger R (1934). "A Relation Between Internuclear Distances and Bond Force Constants" (PDF). *The Journal of Chemical Physics*. 2 (3): 128. Bibcode:1934JChPh...2..128B. doi:10.1063/1.1749433.
22. ^ Hävecker, Michael; Wrabetz, Sabine; Kröhnert, Jutta; Csepei, Lenard-Istvan; Naumann d'Alnoncourt, Raoul; Kolen'Ko, Yury V.; Girgsdies, Frank; Schlögl, Robert; Trunschke, Annette (2012). "Surface chemistry of phase-pure M1 MoVTeNb oxide during operation in selective oxidation of propane to acrylic acid". *J. Catal.* 285: 48–60. doi:10.1016/j.jcat.2011.09.012. hdl:11858/00-001M-0000-0012-1BEB-F.
23. ^ Boosa, Venu; Varimalla, Shirisha; Dumpalapally, Mahesh; Gutta, Naresh; Velisoju, Vijay Kumar; Nama, Narender; Akula, Venugopal (2021-09-05). "Influence of Brønsted acid sites on chemoselective synthesis of pyrrolidones over H-ZSM-5 supported copper catalyst". *Applied Catalysis B: Environmental*. 292: 120177. doi:10.1016/j.apcatb.2021.120177. ISSN 0926-3373.
24. ^ Fajdek-Bieda, Anna; Wróblewska, Agnieszka; Miądlicki, Piotr; Tołpa, Jadwiga; Michalkiewicz, Beata (2021-08-01). "Clinoptilolite as a natural, active zeolite catalyst for the chemical transformations of geraniol". *Reaction Kinetics, Mechanisms and Catalysis*. 133 (2): 997–1011. doi:10.1007/s11144-021-02027-3. ISSN 1878-5204. S2CID 236149569.
25. ^ Azancot, Lola; Bobadilla, Luis F.; Centeno, Miguel A.; Odriozola, José A. (2021-05-15). "IR spectroscopic insights into the coking-resistance effect of potassium on nickel-based catalyst during dry reforming of methane". *Applied Catalysis B: Environmental*. 285: 119822. doi:10.1016/j.apcatb.2020.119822. ISSN 0926-3373. S2CID 232627637.
26. ^ Nuguid, Rob Jeremiah G.; Elsener, Martin; Ferri, Davide; Kröcher, Oliver (2021-12-05). "Operando diffuse reflectance infrared detection of cyanide intermediate species during the reaction of formaldehyde with ammonia over V2O5/WO3-TiO2". *Applied Catalysis B: Environmental*. 298: 120629. doi:10.1016/j.apcatb.2021.120629. ISSN 0926-3373.
27. ^ "Infrared Spectroscopy". *ColourLex*. 12 March 2021. Retrieved 19 January 2022.
28. ^ Derrick MR, Stulik D, Landry JM (2000). "Infrared Spectroscopy in Conservation Science, Scientific Tools for Conservation" (PDF). Getty Publications. Retrieved 11 December 2015.

29. ^ Ricciardi P. "Unlocking the secrets of illuminated manuscripts". Retrieved 11 December 2015.
30. ^ Lau WS (1999). Infrared characterization for microelectronics. World Scientific. ISBN 978-981-02-2352-6.
31. ^ Osborne BG (2006). "Near-Infrared Spectroscopy in Food Analysis". Encyclopedia of Analytical Chemistry. John Wiley & Sons. doi:10.1002/9780470027318.a1018. ISBN 9780470027318.
32. ^ Villar A, Gorritxategi E, Aranzabe E, Fernández S, Otaduy D, Fernández LA (December 2012). "Low-cost visible-near infrared sensor for on-line monitoring of fat and fatty acids content during the manufacturing process of the milk". Food Chemistry. 135 (4): 2756–60. doi:10.1016/j.foodchem.2012.07.074. PMID 22980869.
33. ^ www.TRMThemes.com, TRM Theme by. "Infrared (IR) / Optical Based Archives - Heath Consultants". Heath Consultants. Retrieved 2016-04-12.
34. ^ "NASA Ames PAH IR Spectroscopic Database". The Astrophysics & Astrochemistry Laboratory. 12 September 2019. Retrieved 19 January 2022.
35. ^ Hoover R (February 21, 2014). "Need to Track Organic Nano-Particles Across the Universe? NASA's Got an App for That". NASA. Retrieved February 22, 2014.
36. ^ Becker, Wolfgang; Sachsenheimer, Kerstin; Klemen, Melanie (2017). "Detection of Black Plastics in the Middle Infrared Spectrum (MIR) Using Photon Up-Conversion Technique for Polymer Recycling Process". Polymers. MDPI. 9 (9). doi:10.3390/polym9090435. PMC 6418689. PMID 30965736.
37. ^ Perry, Tekla S. (2017-03-14). "What Happened When We Took the SCiO Food Analyzer Grocery Shopping". IEEE Spectrum: Technology, Engineering, and Science News. Retrieved 2017-03-23.
38. ^ Coates, John (18 June 2014). "A Review of New Small-Scale Technologies for Near Infrared Measurements". American Pharmaceutical Review. Coates Consulting LLC. Retrieved 2017-03-23.
39. ^ Kohli KK, Davies G, Vinh NQ, West D, Estreicher SK, Gregorkiewicz T, et al. (June 2006). "Isotope dependence of the lifetime of the vibration of oxygen in silicon". Physical Review Letters. 96 (22): 225503. Bibcode:2006PhRvL..96v5503K. doi:10.1103/PhysRevLett.96.225503. PMID 16803320.
40. ^ Hamm P, Lim MH, Hochstrasser RM (1998). "Structure of the amide I band of peptides measured by femtosecond nonlinear-infrared spectroscopy". J. Phys. Chem. B. 102 (31): 6123–6138. doi:10.1021/jp9813286.
41. ^ Mukamel S (2000). "Multidimensional femtosecond correlation spectroscopies of electronic and vibrational excitations". Annual Review of Physical Chemistry. 51 (1): 691–729. Bibcode:2000ARPC...51..691M. doi:10.1146/annurev.physchem.51.1.691. PMID 11031297. S2CID 31230696.
42. ^ Demirdöven N, Cheatum CM, Chung HS, Khalil M, Knoester J, Tokmakoff A (June 2004). "Two-dimensional infrared spectroscopy of antiparallel beta-sheet secondary structure" (PDF). Journal of the American Chemical Society. 126 (25): 7981–90. doi:10.1021/ja049811j. PMID 15212548.



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