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 **Studying the vibrational energy levels for some molecules**

RESEARCH PROJECT

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**ABSTRACT**

 Infrared spectroscopy, which is a technique for classifying substances based on the infrared wavelengths they can absorb, can be used to study the energy levels of molecules. On the spectrum, infrared light comes right after visible light.

 The branch of spectroscopy that examines the infrared portion of the electromagnetic spectrum is called infrared spectroscopy, or IR spectroscopy. It includes a variety of methods, the most widely used of which is an absorption spectroscopy variant. It can be used, like all spectroscopic techniques, to determine the composition of samples or identify chemicals. Utilized extensively in both academia and business, infrared spectroscopy is a straightforward and dependable method for measurement, quality assurance, and dynamic assessment. It is very helpful for forensic analysis in civil and criminal situations, allowing for the identification of degradation of polymers, for example. It's probably the most popular applied spectroscopic technique.

In this study, the vibration levels of a few samples were examined, and the energy levels and their differences were computed using a Matlab software that was written.

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**Chapter One: INTRODUCTION**

 Harmonic, pseudo-harmonic, and anharmonic oscillators are important in many areas of physics and have been applied extensively to resolve a variety of physical problems. Much effort is being spent into determining the general formulas for wave functions and vibration-rotation energy spectra in molecular systems in order to achieve that goal. A frequent model and helpful tool for deciphering a range of physical phenomena is the basic harmonic oscillator. This model is one of the fully solvable potentials of the Schrödinger equation and its incorporation into quantum mechanics theory is fundamental to the theory's mathematical formalism (Cohen-Tannoudji, 1986).(Amila et al., 2021)

In contrast, the majority of real-world physical events depend on explicit departures from the harmonic form, necessitating the inclusion of minor non-harmonic components in the description. One real-world issue that lies in between harmonic and anharmonic potentials is the pseudo-harmonic oscillator pattern. This potential's primary characteristic is that it makes it possible to compute molecular vibration-rotation energy spectra in chemical physics(Ikhdair and Hamzavi, 2012). Nevertheless, to restore the agreement between the theory and the data, intrinsic anharmonic effects must be included for real systems.

Generally speaking, it is impossible to obtain a precise solution to such systems; nonetheless, textbooks and research articles frequently provide customary rough answers. (Cohen-Tannoudji, 1986) (Amila et al., 2021) (Kunc and Gordillo-Vazquez, 1997) (Kunc and Gordillo-Vazquez, 1997). Modeling the atomic potential is one of the most essential aspects of molecular dynamics in this regard. Dunham (Dunham, 1929) and Pöschl-Teller (Pöschl and Teller, 1933) are two examples of anharmonic functions that have been devised and employed to solve the Schrödinger equation of these systems. For these systems, the well-known Morse potential function (Burkhardt and Leventhal, 2007) (Morse, 1929) is a more acceptable and realistic model. In this aspect, the Morse potential model is popular among chemists since it accurately describes the observed vibrational energy spectrum of diatomic molecules.

Further exploration of the fundamental formulas of anharmonic potential analysis with the Floquet representation, from which some general results on Morse potentials have been derived, is desired. Muhammad Janati et al. established the explicit wave function to the second order of approximation. (Idrissi et al., 2020). These are realized for the following diatomic molecules (ScN, LiH, Cl2, and NO) in order to determine the finite number of bound states, as well as the dissociation energy and wave functions. Studding vibration energy states can be determined by infrared radiation or infrared spectroscopy.

 The majority of us are familiar with infrared radiation. Meals have been kept warm using infrared lamps, and heat is commonly linked to infrared radiation. It's important to differentiate between heat generation and infrared radiation absorption, even though the latter is most likely the cause. While infrared light can pass through a vacuum, heat is associated with the motion and kinetic energy of molecules. Heat has no relevance because there are no molecules or molecular motion in a vacuum. Infrared spectroscopy is the study of how molecules absorb infrared light and transform it into heat.

By examining how this occurs, we will gain knowledge not only about the absorption of infrared light but also about molecular structure and how infrared spectroscopy can provide insight into the structure of organic molecules. The infrared spectrum of a chemical compound is like a picture of a molecule. On the other hand, unlike a typical image that will show the position of nuclei, the infrared spectrum will only provide a partial structure. Infrared spectroscopy (IR spectroscopy) is the subset of spectroscopy that studies the infrared portion of the electromagnetic spectrum. It covers a range of techniques, the most popular being absorption spectroscopy. (Idrissi et al., 2020)

It can be used to determine the composition of samples or identify substances, just as any other spectroscopic techniques. A typical lab tool that employs this method is the infrared spectrophotometer.

**Chapter Two: THEORY**

**2.1- Regions of Infrared**

The electromagnetic spectrum's near-, mid-, and far-infrared regions are called so based on how they relate to the visible spectrum. With a wavelength range of 400–10 cm-1 (1000–30 m), the far-infrared has low energy and can be used for rotational spectroscopy. It is located near the microwave zone. In the mid-infrared (about 4000–400 cm–1 (30–2.5 m), the fundamental vibrations and related rotational–vibrational structure can be examined. Higher energy near-infrared radiation, approximately 14000–4000 cm-1 (2.5–0.8 m), can trigger overtone or harmonic vibrations. The names and classifications of these subregions are merely guidelines. They are neither tight divisions, nor are they predicated on exact chemical or electromagnetic properties.

**2.2-** infrared absorption

As with UV radiation, the energy of infrared radiation is insufficient to cause electronic changes. Only compounds with small energy differences between their several vibrational and rotational states can absorb infrared radiation.

To absorb infrared radiation, a molecule's dipole moment needs to be changed net by its internal vibrations or rotations. Variations in the dipole moment of the molecule interact with the radiation's alternating electrical field. If the frequency of the radiation coincides with the molecule's vibrational frequency, the molecule will absorb the radiation, changing the amplitude of molecular vibration..(Kunc and Gordillo-Vázquez, 1997)

The fact that molecules spin or vibrate at particular frequencies that correspond to distinct energy levels (vibrational modes) is exploited by infrared spectroscopy. A vibrational mode of a molecule needs to be connected to modifications in the permanent dipole in order for it to be IR active. The resonant frequencies are determined by the normal modes corresponding to the molecular electronic ground state potential energy surface in the Born–Oppenheimer and harmonic approximations, that is, when the molecular Hamiltonian corresponding to the electronic ground state can be approximated by a harmonic oscillator in the vicinity of the equilibrium molecular geometry. (Kunc and Gordillo-Vazquez, 1997)

In a basic diatomic molecule, the solitary bond has the ability to stretch. More complicated molecules can absorb infrared light at particular frequencies that may be linked to chemical groups because they have more bonds and are capable of conjugating vibrations. For instance, as figure (2.1) illustrates, the atoms in a CH2 group are capable of six different types of vibration: symmetrical and anti-symmetrical stretching, scissoring, rocking, wagging, and twisting.



 Figure(2.1):types of molecule vibration

An infrared light beam is sent through a sample to obtain its infrared spectrum. Observing the transmitted light will reveal the quantity of energy absorbed at each wavelength.

**2-3-Vibration of Molecules**

When a body is moved from its equilibrium position and is drawn back toward it by a restoring force, this is known as a vibration. If the potential energy is proportional to the square of the displacement or if the restoring force, F, is proportionate to the displacement, x, the vibration will be harmonic:

 F = -k x or V = 1/2 kx^2

Since force always works in the opposite direction of displacement, the force expression has a minus sign. The "force constant" is the name given to the proportionality constant, k.

When studying molecular vibrations, diatomic molecules will offer the most straightforward example to begin with. It will be observed that the "harmonic approximation" is not totally satisfactory, and the vibration's anharmonicity will be taken into consideration in the following stage. Eventually, the issue of polyatomic molecule vibrations will be addressed using both phases of approximation. (Cohen-Tannoudji, 1986).

 **2.3.1- Harmonic vibrations of diatomic molecules**

By introducing the reduced mass into The Theory of Molecular Structure, it is feasible to convert the "two-body" difficulty posed by a diatomic molecule into a "one-body" one. The mass of each of the two atoms that make up the molecule is m1, and their distance from one another is r. Consult Figure 2-1.

For each x = r – re, let re be the equilibrium distance and ''displacement.''

The potential energy and the restoring force are determined by the definition of harmonicity, which is:

 V = 1/2 k(r – re )2 = 1/2 kx2 (2-1)

 F = -(r – re) = - k x (2-2)

In classical mechanics the motion of the two atoms is governed by the Newton’s equations:

 –k x = m1 d2r1/dt2

 and - k x = m2 d2r2/dt2 (2-3)

 By the properties of the center of mass:

 R1 = r m2/(m1 + m2) r2 = rm1/(m1 + m2) (2-4)

Introducing these values into 2-3, we reduce both equations to the same form:

 -k x = d2r/dt2 or -k x = d2x/dt2 (2-5)

The solution of the differential equation 3-5 is

 x = x m sin (t + ) with =  (2-6)

as may by easily verified by taking the second time derivative. The classical frequency of oscillation is finally obtained:

 *vo* = 1/2  ( 2-7)

As far as the vibration is concerned, the diatomic molecule is equivalent to a single body of mass ***m***oscillating under the influence of a force constant ***k***.if the center of gravity is im mobile, the individual motions of the two atoms may by obtained from equations 2-4. One is more generally concerned with the mode of the inter atomic distance (Amila et al., 2021).

In *quantum mechanics*, acceptable solution of the wave equation are obtained only if the energy takes the following quantized values:

 E[v] = h *vo* (v + 1/2) v = 0, 1, 2,… (2-8)

Where *vo* is the classical frequency of oscillation given by equation 2-7. The *term value* for the vibrational levels is usually represented by **G,** so that:

 G(v) = E/hc = *vo/c* (v +1/2)

 or

 G(v) = w(v + 1/2) v = 0, 1, 2,…. (2-9)

Consequently, the diatomic molecule possesses a series of equidistant energy levels, the lowest having a value E[0] = 1/2 h*vo*, which is called the ''zero-point energy .''

Radiative transitions between those levels are restricted by the following selection rules. In order to be active in infrared, a transition has to satisfy the relation

 v = 1.

In addition, the rate of change of the dipole moment must be different from zero. The selection rule for v is the same for the Raman effect, and here, the polarizability of the molecule must change during the vibration. Let us apply the selection rule to see what kind of absorption spectrum is to be expected from a diatomic molecule. If, as usual , the prime (′) is taken for the upper level and the doublePrime ('') for the lower level, the wave number of the unique line predicted by this theory is:

****  V = G(v') – G(v") with v"= v' - 1

So that

 *V = w=* *vo/c* = 1/2*c * (2-10)

Actually, polar diatomic molecules like CO and HCl have just one strong band in their infrared spectra, and as will be demonstrated below, attributing this band to a vibrational transition yields a plausible estimate for the force constant. Nonetheless, two opposing characteristics are also readily noticeable. First off, the absorption addresses the interaction between rotation and vibration by means of a band, which is a collection of lines rather than a single, isolated line. Second, in addition to the strong band already indicated, other bands may also be detected in the spectrum. Their wave numbers are roughly integral multiples of the fundamental's wave number, and they are referred to as "overtones" of the anticipated or "fundamental" bands.

 The presence and the exact position of these overtones will be explained only by taking into account the anharmonicity of the vibration.(Idrissi et al., 2020)

Limited as it is, the harmonic approximation furnishes, through the wave mechanical treatment, a very useful relation between the observed wave number and the force constant holding the two atoms together in the molecule. For example, the center of the most intense band in the infrared spectrum of HCl is at

 *v* = 2885.9 cm-1

And using this, we calculate the value of the force constant to be:

 K = 4. 8  105 dyne/cm

Such a force constant would give a fairly strong; its expression in the above units has little meaning for a molecule, however, because an increase of 1 centimeter in the inter nuclear distance would break the molecule apart. It would be more realistic to say that an increase of 1/10A requires a force of 1.08  10-9 lb. This may seem very small, but it has to be kept in mind that the masses involved are also exceedingly small. The ''classical'' frequency of oscillation that this force produces is equal to 8.6  1013 cps.

Finding the "classical amplitude" that corresponds to a certain energy level is feasible if one assumes that the complete energy is in the potential at the moment of maximum vibrational displacement.

 Using the previously calculated value of K to estimate the dissociation energy and comparing it to the experimental value provided by chemical measurements is another method of verifying the accuracy of the quantum mechanical results. Assume for the moment that the bond breaks when its length increases by one A. The amount of work required for this increase will represent the dissociation energy, and its value is equal to the variation of potential energy, which is just the value of the potential energy when x = 1A; therefore

 Dissociation energy = 1/2 k =10 -16 erg

This results in a value for HCl of 345 kcal/mole, which is comparable to the experimental value of 103 kcal/mole. Explaining the disparity in the numerical figures is simple. The biggest flaw in this approach is that a harmonic potential creates a restoring force that increases as the interatomic distance increases. To start, determining the distance at which a molecule is deemed to be dissociated is mainly arbitrary. As a result, until the distance is infinite, the dissociation work carried would have a limitless value.

**2.3.2-Anharmonic vibration of diatomic molecules**

It is possible to calculate the precise form of the potential curve controlling the nuclei's vibrational motion. It is the "electronic energy" that the Born-Oppenheimer theorem introduced. Alternatively, it can be fragmentary built from the measured rotational and vibrational levels.

Only very tiny values of x, that is, as long as V = 1/2 k x2 is a reasonable approximation of the actual potential,

The broken line curve is the parabola that creates the best approximation of the real curve at the minimum [harmonic approximation], while the full curve displays the findings of the experiment. The optimal cubic potential function can be seen as the dotted line.(Dunham, 1929)

The internuclear distance **r** remains near its equilibrium value **re.**

Other analytical functions have been proposed, giving a better agreement with the real curve. We will examine only two of them, the *cubic function* and the *Morse function.*

* + 1. **Cubic potential function**

 For a better agreement with the empirical curve, a cubic term may be added to the expression of the potential function:

 V = f (r – re)2 - (r – re)3 (2-11)

If this value is introduced in the wave equation, the following from is obtained for the energy levels (in *term value*):

 G(v) = we (v + 1/2) – we xe [v + 1/2]2 (2-12)

Where we is the *vibrational frequency for infinitesimal amplitude* and has the value:

 We = 1/2c  (2-13)

The ''anharmonic constant'' wexe is much smaller than we, so that the energy levels given by the harmonic approximation are not very different from the ''anharmonic levels,'' the gap, however, increases with the value of v.

The restoring force is the derivative of V in respect to x = r – re:

 F = - dv/dx = - 2fx + 3gx^2

It is no longer proportional to the deformation x, as it was in the harmonic case.

 For infinitesimal amplitudes, however, the cubic term in V may be neglected so that F becomes equal to -2fx . For this reason, 2f is called ''force constant for infinitesimal amplitudes.'' In the *selection rule*, also, the anharmonicity introduces something new. The quantum number v, now, vary by any whole number:

 V =  2, …

It should be remarked that the predicted *intensity* of the lines decreases very rapidly with increasing v . By applying the selection rule to the transitions between the levels given in equation the 3-12, one may calculate the wave numbers of the absorption bands. Some are given in the following formulae:

 *V*1 = G(1) – G(0) = we – 2wexe

*V2 =* G(2) – G(0) = 2we – 6wexe (2-14)

*V*3 = G(3) – G(0) = 3we – 12wexe

The first band is the *fundamental* and the others are the *overtones.* As wexe is nearly always positive, the wave numbers of the overtones are predicted to be smaller than twice, three times, etc., the wave number of the fundamental. This actually the case in the observed spectra, as may be checked on the infrared bands of HCl given below (in cm-1):

*V*1 = 2885.9, *V2* = 5668.0, *V3* = 8346.9, *V4* = 10923.1, *V5 =* 13396.5

With the help of these experimental data, the values of we and we xe may be calculated. Introduced in equation 3-13, the value of we leads to the determination of the force constant for infinitesimal displacements. Another important relation established in the theory of the anharmonic vibrator connects the *dissociation energy* to the vibrational constants [in cm-1]:

 De = we2/4wexe

In the case of HCl, the following values are obtained:

 We = 2989.74 cm-1

 Wexe = 52.05 cm-1

 2f = 5.1574  10^5 dyne/ cm

 De = 4.2932  10^4 cm-1 =122.7 kcal/mole

**2.3.4: The Morse potential function**

 The function

 V = De [1 -  (2-15)

This potential curve, which was proposed by Morse, roughly approximates the true potential of a diatomic molecule, with the exception of r = 0, where the true potential is unlimited and the potential has a finite value. But practically speaking, there is no significance to the portion of the curve that corresponds to very small values of r. The second component of equation 2-15 becomes equal to zero when r = re; this is the smallest potential energy value and happens at the equilibrium position. As a result, the dissociation energy is approached by r V..(Burkhardt and Leventhal, 2007)

**Chapter Three: (Results and Discussion)**

 When the Schrödinger equation is solved using a cubic potential one obtain energy levels of the form: Ev= we(v+1/2) - wexe (v+1/2)2 cm-1

The (wexe) term, called the anharmonicity constant, is positive and much smaller than we, also it’s a product of (we) and (xe), it is unusual to see the (xe) value given separately and we shall use (wexe) as a single number. Because the decreasing separation with increasing v and converge as they approach the dissociation limit. However, unlike the hydrogen atom there is a finite number of such levels leading to dissociation.

We can write the above equation as:

Ev= we [1- xe (v+1/2)].(v+1/2)

Comparison of these two equations one could write:

(Wosc)anh = we[1-xe(v+1/2)]

if we now consider the hypothetical energy state v=-1/2(Ev=0) its oscillation frequency would be given by (wos)anh = we. Thus (we) is the (hypothetical) equilibrium oscillation frequency – the frequency of oscillation for infinitesimal motions about the bottom of the well. We find that the zero point energy of the anharmonic oscillator (v=0) is given by

E0= 1/2 we (1- xe/2) cm-1

**3-1 Determination of harmonic and anharmonic energy levels of (CO) molecule Input parameters for Co Molecule**

n= 12, m=16 Mass number of the first and second atom respectively

we= 2169.81 cm-1 Harmonic constant

xe= 13.288 cm-1, ye= 0.0105 cm-1 Anharmonic constants

output parameters:

M = 1.1391 x10-23 gm Reduced mass for molecule

k = 1.9035 x106 dyne/cm-1 Force constant of the molecule

**Table:(3.1) values of harmonic and anharmonic energy levels and difference between them**.

|  |  |  |  |
| --- | --- | --- | --- |
| **V** | **Harmonic energy(**cm-1) | **Anharmonic energy(**cm-1) | **Anh. spacing(**cm-1) |
| 0 | 1085 | 1082 |  |
| 1 | 3255 | 3225 | 2143 |
| 2 | 5425 | 5342 | 2117 |
| 3 | 7594 | 7432 | 2090 |
| 4 | 9764 | 9496 | 2064 |
| 5 | 11934 | 11534 | 2038 |
| 6 | 14104 | 13545 | 2011 |
| 7 | 16274 | 15531 | 1986 |
| 8 | 18443 | 17490 | 1959 |
| 9 | 20613 | 19423 | 1933 |
| 10 | 22783 | 21330 | 1907 |

Vmax =81

De = 88578 cm-1 Dissociation energy

delEh = 2143.2 cm-1 Fundamental frequency

delEov1 = 4259.9 cm-1 First overtone frequency

delEov2 = 6350.0 cm-1 Second overtone frequency

delEov3 = 8413.5 cm-1 Third overtone frequency

delEov4 = 10450 cm-1 Fourth overtone frequency

delEov5 = 12461 cm-1 Fifth overtone frequency

 From results in table above it appear that with increasing the number of vibration energy levels the difference between energy levels decrease then for large number of energy levels the levels act as continuous as we see that the difference between the first and second level is equal to (2143cm-1), when its equal to(1907cm-1) for difference between levels of ninth and tenth. At the dissociation limit the energy spacing goes to zero, then the vibration level that the molecule dissociate is equal to (81).

**3-2 Determination of harmonic and anharmonic energy levels of H2 molecule**

**Input parameters for H2 Molecule**

 n= 1 , m=1 mass number of the first and second atoms respectively

we= 4401.2 cm-1 harmonic constant

xe= 121.3 cm-1 , ye= 0.812 cm-1 Anharmonic constant

output parameters:

M = 8.3056 x10-25 gm , Reduced mass

 k = 5.7105 x105 dyne/cm-1 Force constant

**Table(3.2): values of harmonic and anharmonic energy levels and difference between them.**

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Harmonic energy** (cm-1) | **Anharmonic energy**(cm-1) | **Anh. Difference** (cm-1) |
| 0 | 2201 | 2170 |  |
| 1 | 6602 | 6332 | 4162 |
| 2 | 11003 | 10258 | 3926 |
| 3 | 15404 | 13953 | 3695 |
| 4 | 19805 | 17423 | 3470 |
| 5 | 24207 | 20672 | 3249 |
| 6 | 28608 | 23706 | 3034 |
| 7 | 33009 | 26528 | 2822 |
| 8 | 37410 | 29145 | 2617 |
| 9 | 41811 | 31560 | 2415 |
| 10 | 46213 | 33779 | 2219 |

Vmax=18

de = 39923 cm-1 Dissociation energy

delEh = 4158.6 cm-1 Fundamental frequency

delEov1 = 8.074.6 cm-1 First overtone frequency

delEov2 = 11748 cm-1 Second overtone frequency

delEov3 = 15179 cm-1 Third overtone frequency

delEov4 = 18367 cm-1 Fourth overtone frequency

delEov5 = 21313 cm-1 Fifth overtone frequency

 From results in table above it appear that with increasing the number of vibration energy levels the difference between energy levels decrease then for large number of energy levels the levels act as continuous as we see that the difference between the first and second level is equal to (4162cm-1), when its equal to(2219cm-1) for difference between levels of ninth and tenth.

**3-3 Determination of harmonic and anharmonic energy levels of HCl molecule Input parameters for HCl molecule**

n= 1 , m=35 Mass number of the first and second atoms respectively

 we= 2990.6 cm-1 Harmonic constant

xe= 52.82 cm-1 , ye= 0.2243 cm-1 Anharmonic constant

 output parameters:

M = 1.6150x10-24 gm Reduced mass

k = 5.1278x105 dyne/cm-1 Force constant

**Table(3.3): values of harmonic and anharmonic energy levels and difference between them.**

|  |  |  |  |
| --- | --- | --- | --- |
| **V** | **Harmonic energy(cm-1)** | **Anharmonic energy(cm-1)** | **Anh.spacing(cm-1)** |
| 0 | 1495 | 1482 |  |
| 1 | 4486 | 4368 | 2887 |
| 2 | 7477 | 7151 | 2784 |
| 3 | 10468 | 9831 | 2682 |
| 4 | 13459 | 12410 | 2581 |
| 5 | 16450 | 14889 | 2480 |
| 6 | 19441 | 17271 | 2380 |
| 7 | 22432 | 19555 | 2281 |
| 8 | 25423 | 21744 | 2183 |
| 9 | 28414 | 23839 | 2085 |
| 10 | 31404 | 25841 | 1988 |

Vmax=28

 De = 42339 cm-1 Dissociation energy

 delEh = 2885.3 cm-1 , Fundamental frequency

 delEov1 = 5664.9 cm-1 First overtone frequency

delEov2 = 8338.9 cm-1 Second overtone frequency

 delEov3 = 10907 cm-1 Third overtone frequency

delEov4 = 13370 cm-1 Fourth overtone frequency

delEov5 = 15727 cm-1 Fifth overtone frequency

**3-4 Determination of harmonic and anharmonic energy levels of HF molecule Input parameters for HF Molecule.**

n = 1 , m = 19 Mass number of the first and second atom respectively

we = 4138.5 cm-1 Harmonic constant

xe = 90.21 cm-1 , ye= 0.55 cm-1 Anharmonic constant

output parameters:

M =1.57 x10-24 gm Reduced mass,

 k = 9.5935 x105 dyne/cm-1 Force constant

**Table(3.4): values of harmonic and anharmonic energy levels and difference between them**

|  |  |  |  |
| --- | --- | --- | --- |
| V | **Harmonic energy (cm-1)** | **Anharmonic energy(cm-1)** | **Anh. Spacing (cm-1)** |
| 0 | 2069 | 2047 |  |
| 1 | 6208 | 6007 | 3960 |
| 2 | 10346 | 9791 | 3784 |
| 3 | 14485 | 13403 | 3612 |
| 4 | 18623 | 16847 | 3444 |
| 5 | 22762 | 20124 | 3277 |
| 6 | 26900 | 23240 | 3116 |
| 7 | 31039 | 26196 | 2956 |
| 8 | 35177 | 28997 | 2649 |
| 9 | 39316 | 31646 | 2537 |
| 10 | 43454 | 34145 | 2499 |

Vmax=22

De = 47465 cm-1 Dissociation energy

delEh = 3958.1 cm-1 Fundamental frequency

delEov1 = 7735.7 cm-1 First overtone frequency

delEov2 = 11333 cm-1 Second overtone frequency

delEov3 = 14750 cm-1 Third overtone frequency

delEov4 = 17986 cm-1 Fourth overtone frequency

delEov5 = 21042 cm-1 Fifth overtone frequency

**4- Conclusion**

In conclusion, the study focused on investigating the vibrational energy levels of selected molecules, shedding light on the complicated dynamics within molecular structures. Through the application of spectroscopic techniques, such as infrared spectroscopy, the research aimed to distinguish and analyze the vibrational modes exhibited by these molecules.

The vibrational energy levels play a pivotal role in understanding the internal motion and stability of molecules, providing valuable insights into their structural characteristics and potential reactivity. By probing the vibrational signatures, this study has contributed to the broader field of molecular spectroscopy, advancing our comprehension of the fundamental principles governing molecular behavior.

results for all previous samples indicate that vibration lines are approach to each other by increasing the number of energy vibration level it mean that with increasing the number of energy vibration level the difference between levels will decrease.

**5-References**

AMILA, I., IDRISSI, M., FEDOUL, A. & SAYOURI, S. 2021. An approach to determine the diatomic vibrational energy levels: application to LiH, NO and CO molecules. *IOP Conference Series: Materials Science and Engineering,* 1160**,** 012003.

BURKHARDT, C. E. & LEVENTHAL, J. J. 2007. Vibration-rotation coupling in a Morse oscillator. *American Journal of Physics,* 75**,** 686-689.

COHEN-TANNOUDJI, C. D. B. L. F. 1986. *Me��canique quantique. Tome II Tome II*.

DUNHAM, J. L. 1929. Intensities in the Harmonic Band of Hydrogen Chloride. *Physical Review,* 34**,** 438-452.

IDRISSI, M., FEDOUL, A., SAYOURI, S. & AMILA, I. 2020. Anharmonic Potentials Analysis through the Floquet Representation. *Journal of Applied Mathematics and Physics,* 08**,** 184-195.

IKHDAIR, S. M. & HAMZAVI, M. 2012. Approximate Relativistic Bound State Solutions of the Tietz–Hua Rotating Oscillator for Any κ-State. *Few-Body Systems,* 53**,** 473-486.

KUNC, J. A. & GORDILLO-VAZQUEZ, F. J. 1997. Rotationaé Vibrational Levels of Diatomic Molecules Represented by the Tietú Hua Rotating Oscillator. *Journal of Physical Chemistry A,* 101**,** 1595-1602.

KUNC, J. A. & GORDILLO-VÁZQUEZ, F. J. 1997. Rotational−Vibrational Levels of Diatomic Molecules Represented by the Tietz−Hua Rotating Oscillator. *The Journal of Physical Chemistry A,* 101**,** 1595-1602.

MORSE, P. M. 1929. Diatomic Molecules According to the Wave Mechanics. II. Vibrational Levels. *Physical Review,* 34**,** 57-64.

PÖSCHL, G. & TELLER, E. 1933. Bemerkungen zur Quantenmechanik des anharmonischen Oszillators. *Zeitschrift für Physik,* 83**,** 143-151.

**Appendix I**

% Parameters

D = 4.0; % Dissociation energy (in eV)

a = 0.1; % Morse potential parameter (in Å^-1)

x\_min = 0; % Minimum bond length (in Å)

x\_max = 10; % Maximum bond length (in Å)

num\_points = 1000; % Number of points for calculation

% Harmonic potential

V\_harmonic = @(x) 0.5 \* D \* a^2 \* (x - x\_min).^2;

% Anharmonic potential (Morse potential)

V\_anharmonic = @(x) D \* (1 - exp(-a \* (x - x\_min))).^2;

% Calculate energy levels

x\_values = linspace(x\_min, x\_max, num\_points);

energy\_levels\_harmonic = V\_harmonic(x\_values);

energy\_levels\_anharmonic = V\_anharmonic(x\_values);

% Plotting figure;

plot(x\_values, energy\_levels\_harmonic, 'b', 'LineWidth', 2);

hold on;

plot(x\_values, energy\_levels\_anharmonic, 'r--', 'LineWidth', 2);

xlabel('Bond Length (Å)');

ylabel('Energy (eV)');

title('Harmonic vs Anharmonic Potential Energy');

legend('Harmonic', 'Anharmonic', 'Location', 'Best');

grid on; hold off