Research Article

The Mechanism of Formation of the Vibrational-Rotational Spectrum of the HCL Molecule

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Abstract

In this work, the harmonic and anharmonic vibrational frequencies of the HCl molecule have been determined by using the density functional theory method. Calculations have been performed at the B3LYP/6-311++G (3dp, 3df) levels of theory. Transitions between energy levels are analyzed in terms of wavenumber. The rotational constants of the HCl molecule, the wavenumbers corresponding to the rotational structure of the P, R, and Q branches in the spectrum, and their relative intensities at temperatures of 100, 200, and 300 K are calculated, and vibrational-rotational spectra are simulated. The vibrational-rotational spectrum of the HCl molecule is obtained in the range of 2600-3100 cm^{-1}. It has been theoretically shown that when the distance between atomic nuclei in the HCl molecule increases compared to the steady state, the R branch in the spectrum, and when it decreases, the P branch is formed. Rotational constants and corresponding frequencies are calculated for each fundamental transition in rotational energy levels. All calculations use empirical and non-empirical methods. For $H^{35}Cl$ and $H^{37}Cl$ molecules, graphs of the number of fundamental transitions (m) in rotational energy levels and the wave number corresponding to these transitions are drawn. It is in good agreement with all scale experiment results. It is verified that the rotational constants (B) corresponding to the general degree of degeneration $(2J+1)^2$ are similar to the values observed in the literature.

Keywords

Harmonic, Anharmonicity, Statistical Weight, Hydrogen Chloride, Vibrational-Rotational

1. Introduction

Many problems related to the analysis of the vibrational-rotational spectra of polar diatomic molecules can be solved in different ways. We know that the spectra of polyatomic molecules are complex, and in order to simplify their complexity, we study the spectral parameters of diatomic molecules. Compared to other polar diatomic molecules, the structural structure of the vibrational-rotational spectrum of HCl is different due to the isotope of chlorine, and we consider the effect of this difference on its spectral parameters. Below, we describe an alternative approach to analyzing the vibra-tional-rotational spectrum of the HCl molecule. As an example, consider the analysis of the vibrational-rotational IR spectrum of the hydrogen chloride (or $H^{35}Cl$ and $H^{37}Cl$) molecule for fundamental transitions. [1-7].

Theoretical calculations are the most statistically optimal method of evaluating spectral data and simultaneously analyzing it, as well as determining spectral parameters. As noted by the authors of Reference 6, we use the method of quantification or graphing data to compare the differences between experimentally observed values and theoretically calculated

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values. In article [6], however, a method for the determination of parameter uncertainties in nonlinear fits is described that relies on numerically finding the partial derivatives of the fitting function with respect to the parameters using finite differences.

The method of combination differences [8] is also considered one of the most convenient methods for calculating wave numbers. Using equations 2, 3, and 4, a statistical method capable of giving results similar to the direct fit values I have shown in this work.

The undergraduate physical chemistry experiment [9] of analyzing the infrared spectrum of gas-phase HCl is unequal at illustrating how the vibrational-rotational spectrum reveals molecular structure. These have the advantage of helping to understand the fit between experimental data and a theoretical model.

According to Joel Tellinghuisen et al. [10], the local approach typically deals with subsets of the data treated in similar ways, with the results often subjected to subsequent analysis to arrive at a set of final parameters.

Figure 1. *J'', J' and υ'', υ' are lower and upper rotation quantum numbers and vibrational quantum numbers, respectively; m is the number of transitions between rotational energy levels.*

Figure 1 shows the mechanism of formation of P, Q, and R branches at vibrational-rotational energy levels. In this figure, we have marked the rotational peaks in the spectrum with the letter m and included the transitions between the rotational energy levels corresponding to those peaks.

From the review of the literature, it can be seen that the vibrational-rotational IR spectrum of the HCl molecule has not been sufficiently analyzed. In this study, the temperature dependence of the relative intensity of the HCl molecule, the

wavelengths of some points that do not appear in the spectrum and Q branch, and the change in distance between the nuclei corresponding to the transitions between the rotational energy levels were determined using theoretical calculations.

Computational details

Quantum-chemical calculations Harmonic and anharmonic vibrational frequencies were calculated using the Gaussian 09W program (B3LYP/6-311++G(3df, 3pd)).

Anharmonic vibration frequency and wavenumbers were determined using expressions (2) and (3).

In this work, the rotational constants of the molecule, the vibrational-rotational interaction constant, and, based on the vibrational quantum number and rotational quantum number, the wavenumbers and absorption intensities corresponding to the transitions between the rotational energy levels of the vibrational-rotational spectrum were calculated based on the following formulas:

$$B_{\vartheta} = B_e + \alpha_e (\vartheta + \frac{1}{2}),\qquad(1)$$

The B-rotational constant during vibration-rotational motion depends on the υ-vibration quantum number [11], i.e. Here, α_e is the vibrational-rotational interaction constant.

For diatomic molecules, we use the following formulas [12] to determine the wave numbers corresponding to the transitions of R and P branches between rotational energy levels in the vibrational-rotational spectrum:

$$\tilde{\nu}_R = \tilde{\nu}_0 + 2B' + (3B' - B'')J'' + (B' - B'')J''^2,\qquad(2)$$

$$\tilde{\nu}_P = \tilde{\nu}_0 - 2B'' - (3B'' - B')J' + (B' - B'')J'^2,\qquad(3)$$

Where B'' and B' are the rotational constants of the lower and upper energy levels, respectively.

The wavenumbers corresponding to the rotational transitions of the branch Q can be determined as follows:

$$J'' = J', \quad \tilde{\nu}_{J''\to J'} = \tilde{\nu}_{0\to 0} + (B' - B'')J(J+1),\qquad(4)$$

The formula for determining some wave numbers that do not appear in the spectrum, that is, whose intensities are equal to zero:

$$\tilde{\nu}_n = \tilde{\nu}_{0\to 0} + 2Bn, \quad B = \frac{B' + B''}{2},\qquad(5)$$

For R branch n = 1, 2, 3,..., and for P branch n = -1, -2, -3,...

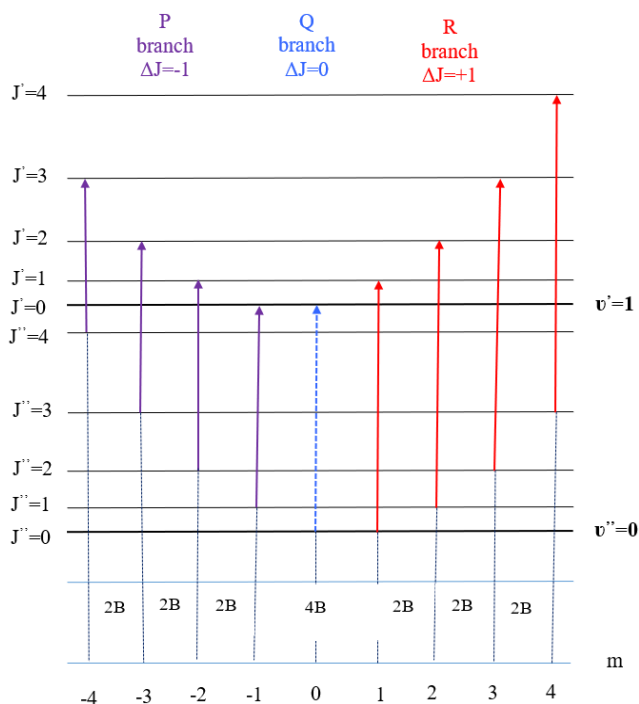The intensity of absorption depends on the statistical weight, which is determined using the following formula:

$$I_{abs.} = \frac{C_{abs.} \tilde{\nu} N}{q} \left(\frac{\sum\limits_{i,j} \left| R^{m_i n_j} \right|}{2J+1} \right) (2J+1) e^{-\frac{E_R}{k_B T}}, \quad (6)$$

where C_{abs} is a constant, ν is the frequency of radiation associated with the transition, R^{mn} is the transition moment integral over the degeneracy i and j in lower and upper states m and n, and the remaining factors occur as a result of solving E_R. 1 for N_J, the population of each rotational state in the lower level. When the assumption is made that the transition probability is the same for all transitions between the $(2J+1)$ degenerate states, the sum of the transition moment integrals equals a constant time, the factor $(2J+1)$. The constant is incorporated into C_{abs}, and the parenthetical term involving R^{mn} then collapses to the value 1, where N is the total number of HCl molecules in the sample, J is the rotational quantum number associated with the $\nu = 0$ vibrational ground state, E_R is the rotational energy of level J, k_B is Boltzmann's constant, T is the absolute temperature, and q is the rotational partition function.

The relative intensity is obtained relative to the peak absorption intensity corresponding to the rotational structures in the spectrum.

2. Results and Discussion

2.1. Observed and Calculated Values.

An FT-IR spectrometer is a spectroscopic instrument that captures high-resolution spectra. This device was used to analyze the spectral lines of vibrational-rotational transitions between energy levels involving the HCl molecule and chlorine isotopes (^{35}Cl and ^{37}Cl). Calculations were analyzed based on this experiment [13].

The calculated harmonic and anharmonic wavenumbers of the $H^{35}Cl$ molecule were found to be 2945.1 and 2890.2 cm^{-1}, respectively. taking k-force constant as constant, $\tilde{\nu}_0(H^{37}Cl)/\tilde{\nu}^{anh}_0(H^{35}Cl)$ through ratio $\tilde{\nu}_0(H^{37}Cl)$=2887,9 cm^{-1} being and reduced masses $\mu(H^{35}Cl)$=1.6359*10^{-24} g, $\mu(H^{37}Cl)$=1.6384*10^{-24} g were calculated. Assuming that the bond length is the same for the ground and first excited states, the difference between the J"=1, v"=0 → J'=0, v'=1 transition and the J"=0, v"=0 → J'=1, v'=1 transition frequencies can be used to estimate the bond length. The separation between the two illustrated vibration-rotation transitions is assumed to be twice the rotational energy change from J"=0 to J'=1. Taking into account that the frequency difference from the vibrational-rotational IR spectrum observed in the experiment [14] is $\Delta\nu(H^{35}Cl)$=41.2 cm^{-1}, $\Delta\nu(H^{37}Cl)$=41.3 cm^{-1}, the distances between the nuclei are r($H^{35}Cl$)=1.286 Å, r($H^{37}Cl$)=1.283 Å, values of rotational constants $B_e(H^{35}Cl)$=10.3497 cm^{-1}, $B_e(H^{37}Cl)$=10.3819 cm^{-1} were found. When calculated using expression (1) using the vibrational-rotational interaction constant α_e =0.303 (taken as constant for $H^{35}Cl$ and $H^{37}Cl$), the rotation for the lower energy level when the vibrational quantum number υ=0 constants $B^{\parallel}(H^{35}Cl)$=10.1982 cm^{-1}, $B^{\parallel}(H^{37}Cl)$=10.2304 cm^{-1}, and for the high energy level at υ=1 ($H^{35}Cl$)=9.8952 cm^{-1}, ($H^{37}Cl$)=9.9274 cm^{-1}, it turned out to be. Tables 1 and 2 below show the transitions between the rotational energy levels of $H^{35}Cl$ and $H^{37}Cl$ molecules, the experimentally observed and calculated wave numbers, and the values of their relative intensities at different temperatures:

Table 1. The calculated wavenumbers ($\tilde{\nu}$, cm^{-1}) and relative intensity (η, %) of the $H^{35}Cl$ molecule at different temperatures.

Peak m	Experi-ment $\tilde{\nu}$	Theory $\tilde{\nu}$	η T=100 K	T=200 K	T=300 K
11	3073,3	3074,6	1,56E-06	0,002684	0,029823
10	3059,4	3060,8	2,42E-05	0,010028	0,069345
9	3045,1	3046,5	0,000279	0,032132	0,145001
8	3029,2	3031,6	0,002386	0,088048	0,271889
7	3013,3	3016,0	0,015072	0,205499	0,455326
6	2997,4	2999,8	0,069934	0,406088	0,676961
5	2980,7	2983,1	0,236017	0,672915	0,884975
4	2962,4	2965,7	0,569540	0,919196	1
3	2944,7	2947,8	0,949435	1	0,943644
2	2925,7	2929,2	1	0,792444	0,680123

Peak m	Experi-ment	Theory			
		η			
	$\tilde{v}$	$\tilde{v}$	T=100 K	T=200 K	T=300 K
1	2906,0	2910,0	0,440138	0,302534	0,247627
-1	2864,8	2869,8	0,434058	0,298355	0,244207
-2	2843,3	2848,8	0,964244	0,767394	0,659566
-3	2821,2	2827,2	0,887453	0,946824	0,897306
-4	2798,8	2805,0	0,511650	0,847296	0,929722
-5	2775,7	2782,2	0,202024	0,601244	0,802104
-6	2751,9	2758,7	0,056547	0,350176	0,596409
-7	2727,7	2734,7	0,011413	0,170280	0,388791
-8	2702,6	2710,1	0,001677	0,069802	0,224350
-9	2677,9	2684,8	0,000181	0,024265	0,115283
-10	2651,8	2659,0	1,43E-05	0,007182	0,052967

Table 2. *The calculated wavenumbers ($\tilde{v}$, cm^{-1}) and relative intensity (η, %) of $H^{37}Cl$ molecule at different temperatures.*

Peak m	Experiment	Theory			
		η			
	$\tilde{v}$	$\tilde{v}$	T=100 K	T=200 K	T=300 K
11	3072,3	3073,0	4,82E-07	0,000849	0,009509
10	3057,8	3059,2	7,54E-06	0,003185	0,022179
9	3042,7	3044,8	8,76E-05	0,010249	0,046505
8	3027,6	3029,8	0,000755	0,028187	0,087414
7	3011,7	3014,2	0,004798	0,066000	0,146708
6	2995,6	2998,0	0,022379	0,130786	0,218526
5	2978,7	2981,2	0,075861	0,217216	0,286106
4	2960,8	2963,7	0,183708	0,297254	0,323682
3	2942,4	2945,7	0,307054	0,323822	0,305713
2	2923,5	2927,2	0,323993	0,256856	0,220483
1	2904,4	2907,8	0,142718	0,098099	0,080295
-1	2863,1	2867,4	0,140735	0,096736	0,079180
-2	2840,9	2846,3	0,312306	0,248688	0,213777
-3	2818,6	2824,7	0,286846	0,30655	0,290651
-4	2796,4	2802,4	0,164864	0,273933	0,300858
-5	2772,6	2779,5	0,064828	0,194015	0,259228
-6	2749,5	2756,0	0,018053	0,112736	0,192450

| Peak m	Experiment	Theory			
		η			
	$\tilde{v}$	$\tilde{v}$	T=100 K	T=200 K	T=300 K
-7	2725,7	2731,9	0,003621	0,054666	0,125217
-8	2701,1	2707,2	0,000528	0,022335	0,072096
-9	2675,6	2681,9	5,64E-05	0,007735	0,036955
-10	2650,2	2656,0	4,42E-06	0,002280	0,016931

As we know, according to the selection rule for transitions between rotational energy levels, the intensities of $\Delta J=0$ transitions do not appear in the vibrational-rotational IR spectrum. Also, using the above expression (4), the values of the calculated wavenumbers corresponding to the Q branch in the spectrum are given in Table 3 below:

Table 3. When J''=J', the wave numbers of J''→ J' transitions of the HCl molecule.

| $\tilde{v}_{J''\to J'}$	$\tilde{v}_{1\to1}$	$\tilde{v}_{2\to2}$	$\tilde{v}_{3\to3}$	$\tilde{v}_{4\to4}$	$\tilde{v}_{5\to5}$	$\tilde{v}_{6\to6}$	$\tilde{v}_{7\to7}$	$\tilde{v}_{8\to8}$	$\tilde{v}_{9\to9}$
$H^{35}Cl$	2889,6	2888,4	2886,6	2884,1	2881,1	2877,5	2873,2	2868,4	2862,9
$H^{37}Cl$	2887,3	2886,1	2884,3	2881,8	2878,8	2875,2	2870,9	2866,1	2860,6
$\tilde{v}_{J''\to J'}$	$\tilde{v}_{10\to10}$	$\tilde{v}_{11\to11}$	$\tilde{v}_{12\to12}$	$\tilde{v}_{13\to13}$	$\tilde{v}_{14\to14}$	$\tilde{v}_{15\to15}$	$\tilde{v}_{16\to16}$	$\tilde{v}_{17\to17}$	$\tilde{v}_{18\to18}$
$H^{35}Cl$	2856,9	2850,2	2842,9	2835,1	2826,6	2817,5	2807,8	2797,5	2786,6
$H^{37}Cl$	2854,6	2847,9	2840,6	2832,8	2824,3	2815,2	2805,5	2795,2	2784,3
$\tilde{v}_{J''\to J'}$	$\tilde{v}_{19\to19}$	$\tilde{v}_{20\to20}$	$\tilde{v}_{21\to21}$	$\tilde{v}_{22\to22}$	$\tilde{v}_{23\to23}$	$\tilde{v}_{24\to24}$	$\tilde{v}_{25\to25}$	$\tilde{v}_{26\to26}$	$\tilde{v}_{27\to27}$
$H^{35}Cl$	2775,1	2762,9	2750,2	2736,9	2722,9	2708,4	2693,3	2677,5	2661,1
$H^{37}Cl$	2772,8	2760,6	2747,9	2734,6	2720,6	2706,1	2691	2675,2	2658,8

In the vibrational-rotational IR spectra of diatomic molecules, the distance between the peaks corresponding to two adjacent rotational transitions is $2B_e$, and these areas are not visible in the spectrum. Using expression (5), the wave numbers in those areas are given in Table 4. Here, n are points that do not appear in the spectrum.
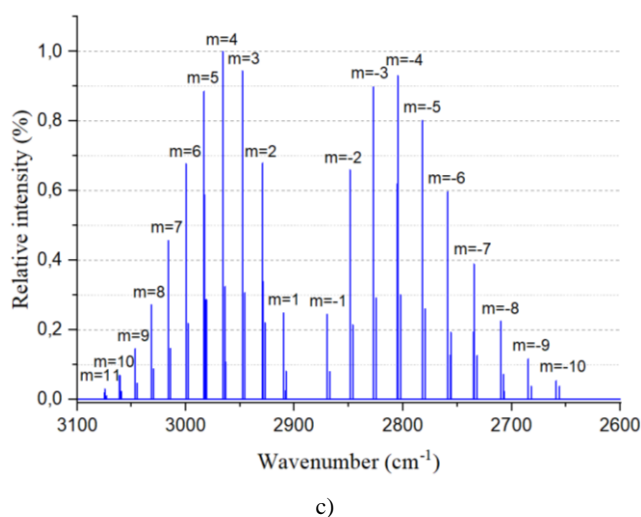

a)

b)

c)
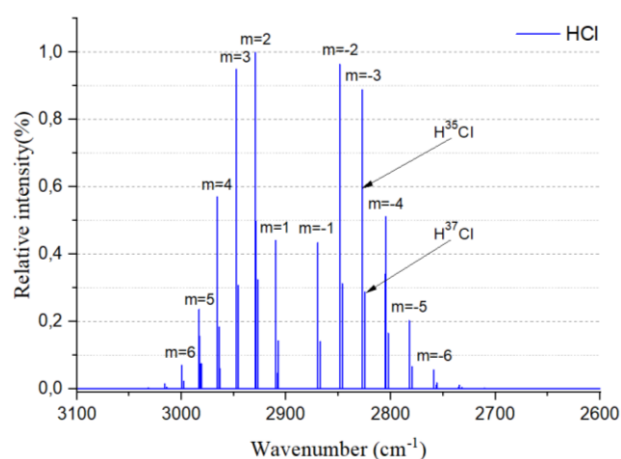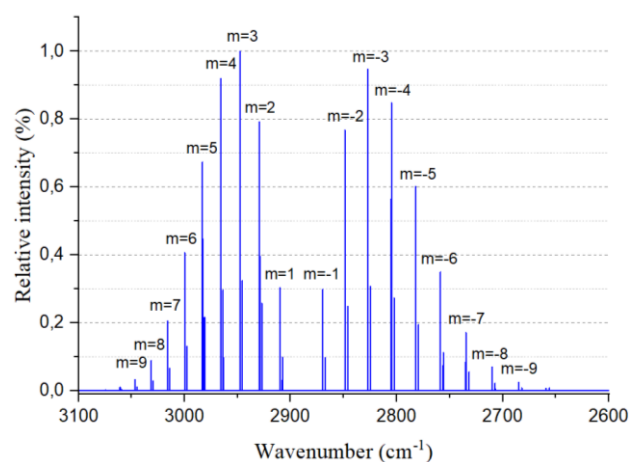
Figure 2. Calculated vibrational-rotational IR spectrum of the HCl molecule: a) T = 100 K; b) T = 200 K; c) T = 300 K.

Table 4. Some wavenumbers do not appear in the vibrational-rotational spectrum of the HCl molecule.

$\tilde{v}_n$	cm^{-1}	
	H^{35}Cl	H^{37}Cl
$\tilde{v}_1$	2910,3	2908,1
$\tilde{v}_2$	2930,4	2928,2
$\tilde{v}_3$	2950,5	2948,4
$\tilde{v}_4$	2970,6	2968,5
$\tilde{v}_5$	2990,7	2988,7
$\tilde{v}_6$	3010,8	3008,8
$\tilde{v}_7$	3030,9	3029,0
$\tilde{v}_8$	3051,0	3049,2
$\tilde{v}_9$	3071,0	3069,3
$\tilde{v}_{10}$	3091,1	3089,5
$\tilde{v}_{-1}$	2870,1	2867,7
$\tilde{v}_{-2}$	2850,0	2847,6
$\tilde{v}_{-3}$	2829,9	2827,4
$\tilde{v}_{-4}$	2809,8	2807,3
$\tilde{v}_{-5}$	2789,7	2787,1
$\tilde{v}_{-6}$	2769,6	2767,0
$\tilde{v}_{-7}$	2749,5	2746,8

$\tilde{v}_n$	cm^{-1}	
	H^{35}Cl	H^{37}Cl
$\tilde{v}_{-8}$	2729,5	2726,6
$\tilde{v}_{-9}$	2709,4	2706,5
$\tilde{v}_{-10}$	2689,3	2686,3
$\tilde{v}_{-11}$	2669,2	2666,2

2.2. Temperature Dependence of the Calculated Vibrational-Rotational Spectrum

The calculated vibrational-rotational IR spectrum of the HCl molecule is shown in Figures 2 a, b, and c in the range from 2600 to 3100 cm^{-1} using the above tables. The relative intensities of the transitions between the rotational energy levels are obtained with respect to the absorption intensity at the maximum height. Here we can observe the effect of three (100, 200, and 300 K) temperatures on the vibrational-rotational IR spectrum. When the temperature is 100 K, the relative intensity of the maximum peak of transitions between rotational energy levels is m=2 (m=3 at T=200 K and m=4 at T=300 K), and the and the vibrational-rotational spectrum 7>m>-7 (10>m>-10 at T=200 K and 12>m>-12 at T=300 K) corresponds to the interval. Finite-temperature anharmonic effects act to broaden and shift the 0 K harmonic peaks while also adding new combination bands.

These effects become more pronounced with increasing temperatures. It also shows two sets of peaks due to H^{35}Cl and H^{37}Cl.

The spacing between the absorption bands is expected to be 2B$_e$ in the P and R branches and 4B$_e$ in the zero gap (Q branch). As can be seen from the spectra, as it moves away from the Q peak, the absorption bands in the P peak move away from each other, while in the R peak they move closer together.

The variation in the vibration spectrum in the Gaussian program is caused by rotational motion and centrifugal disturbance. Spectral numbers and wavenumbers of transitions between calculated rotational energy levels can be found in Tables 1 and 2 at the top of the appendix, and Figures 3a) and b) below show graphs of trends between observed and calculated values. Then, the calculated distance trends of 2B$_e$ and 4B$_e$ match the observed distance trends. The maxima of each absorption band are plotted against the number of passes, as shown in Figure 1.
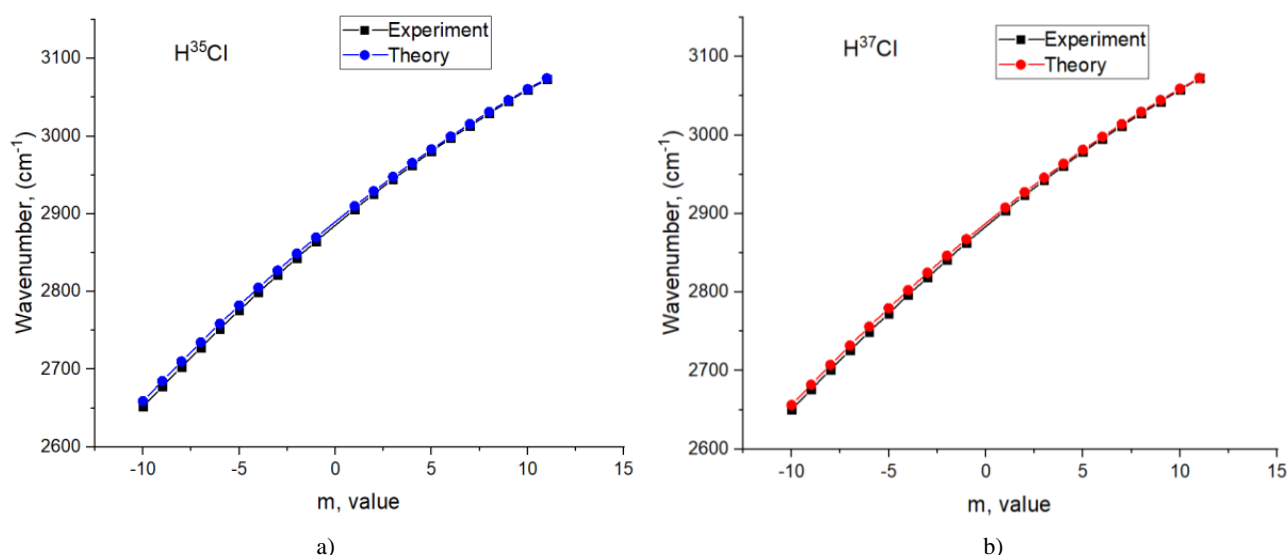
Figure 3. The relationship between wavenumber and transition numbers (m) corresponds to rotational bands in the vibrational-rotational spectrum of the $H^{35}Cl$ (a) and $H^{37}Cl$ (b) molecules.

As can be seen from the spectra in Figure 2, the distances between the peaks corresponding to the transitions between the rotational energy levels decrease from the P branch to the R branch.

The values of this are determined by the difference of the wave numbers corresponding to the transitions between rotational energy levels in the spectra $\Delta\tilde{v}=|\tilde{v}_n-\tilde{v}_{n+1}|$ (n=0,1,2,…), which is determined in cm^{-1} and is given in Table 5 below.

Table 5. Experience and theory of HCl molecules with a rotation constant (B, sm^{-1}) and a general degree of degeneration $(2J+1)^2$.

Peak m	$(2J+1)^2$	Experiment		Theory	
		$2B_H{}^{35}Cl$	$2B_H{}^{37}Cl$	$2B_H{}^{35}Cl$	$2B_H{}^{37}Cl$
11	529	13,9	14,5	13,8	13,8
10	441	14,3	15,1	14,3	14,4
9	361	15,9	15,1	14,9	15,0
8	289	15,9	15,9	15,6	15,6
7	225	15,9	16,1	16,2	16,2
6	169	16,7	16,9	16,7	16,8
5	121	18,3	17,9	17,4	17,5
4	81	17,7	18,4	17,9	18,0
3	49	19,0	18,9	18,6	18,7
2	25	19,7	19,1	19,2	19,2
1	9	20,1	20,5	19,8	19,9
-1	9	21,1	20,8	20,4	20,5
-2	25	21,5	22,2	21,0	21,1
-3	49	22,1	22,3	21,6	21,6
-4	81	22,4	22,2	22,2	22,3
-5	121	23,1	23,8	22,8	22,9

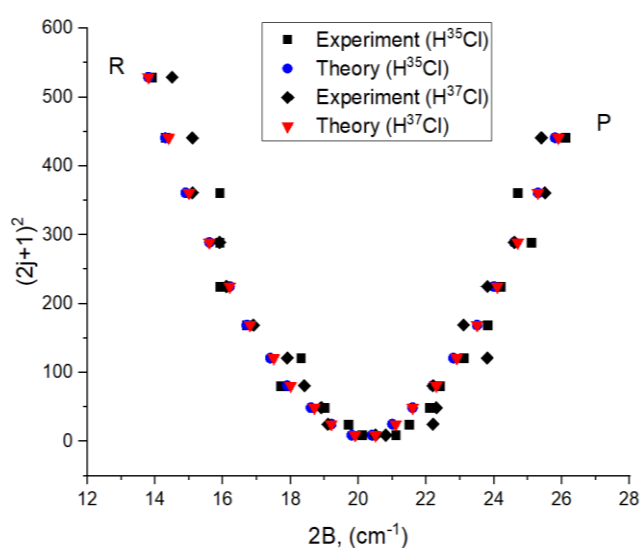| Peak m	$(2J+1)^2$	Experiment		Theory	
		$2B_H{}^{35}Cl$	$2B_H{}^{37}Cl$	$2B_H{}^{35}Cl$	$2B_H{}^{37}Cl$
-6	169	23,8	23,1	23,5	23,5
-7	225	24,2	23,8	24,0	24,1
-8	289	25,1	24,6	24,6	24,7
-9	361	24,7	25,5	25,3	25,3
-10	441	26,1	25,4	25,8	25,9

Figure 4. Graphics of experimentally and theoretically determined $2B_e$ and $(2J+1)^2$.

We look at the total degeneracy levels $((2J+1)^2)$ in this table

as the dependence graph (Figure 4) on the values of the [15] rotation constant $(2B_e)$. We can observe that with an increase in the value of $(2j+1)^2$ in the R branch, the value of $2B_e$ decreases, and for the P branch, the value of $2B_e$ also increases with an increase in the total degeneracy levels. Then the graph will look like a parabola. From this, it can be observed that the energy of the transitions between the energy levels belonging to the R and P branches takes equal values at certain times. It has been calculated that $H^{35}Cl$ and $H^{37}Cl$ change the distances between nuclei [16], corresponding to each circular structure of molecules in the IQ spectrum (Table 6). Vibration-rotation time of the HCl molecule from the steady state: when the distance between the nuclei increases (Figure 5a), the R branch in the spectrum, or vice versa, when it shrinks (Figure 5b), the rotating structures of the P branch bands are formed.

Figure 5. The increase (a) and decrease (b) of the distance between the nuclei of the HCl molecule are shown.

Table 6. *Internuclear distances (r, Å) corresponding to rotational structures in the vibrational-rotational IR spectrum of the HCl molecule were calculated.*

m	1	2	3	4	5	6	7	8	9	10	11
$r_{(H}{}^{35}{}_{Cl)}$	1,315	1,335	1,357	1,383	1,403	1,432	1,454	1,481	1,516	1,547	1,575
$r_{(H}{}^{37}{}_{Cl)}$	1,311	1,334	1,352	1,378	1,398	1,426	1,453	1,480	1,510	1,541	1,574
m	-1	-2	-3	-4	-5	-6	-7	-8	-9	-10	-
$r_{(H}{}^{35}{}_{Cl)}$	1,295	1,276	1,259	1,242	1,225	1,207	1,194	1,180	1,163	1,152	-
$r_{(H}{}^{37}{}_{Cl)}$	1,291	1,273	1,258	1,238	1,222	1,206	1,191	1,176	1,162	1,149	-

When the HCl molecule rotates, the distance between its nu-   clei increases (decreases), and the moment of inertia also

increases (decreases).

Since the constant of rotation is inversely proportional to the moment of inertia of the molecule, its numerical value decreases (increases), and this causes the distance between the rotating structures to decrease towards the higher frequency in the R branch of the spectrum and increase to the lower frequency in the P branch.

3. Conclusions

In this study, the agreement between experiment and theory with finite differences was proved in the graph of the relationship between the frequencies corresponding to the transitions between the rotational energy levels and the number (m) of those transitions.

We can observe that the value of the rotation constant is different at each vibrational level; that is, its value decreases as it rises to the higher vibrational levels.

Since the graph of total degeneracy levels and $2B_e$ is a parabola, it is possible to construct a quadratic function with respect to the rotational quantum number J.

When the HCl molecule rotates, the effect of the change in the distance between the nuclei on the vibrational-rotational spectrum is proven.

It can be seen that the mechanism of formation of vibrational-rotational spectra of similar polar diatomic molecules (HF, CO, HBr, HJ, etc.) is almost the same.

Abbreviations

HCl	Hydrogen Chloride
FT-IR	Fourier Transform Infrared Spectroscopy
IR	Infrared Spectroscopy
T	Temperature

Author Contributions

Gulshan Nurmurodova: Methodology, Investigation, Writing - original draft, Writing - review & editing, Visualization

Utkir Khujamov: Conceptualization, Software, Formal analysis, Writing - original draft, Writing - review & editing, Visualization

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Conflicts of Interest

The authors declare no conflicts of interest.

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