Determination and study the energy characteristics of vibrational-rotational levels and spectral lines of GaF, GaCl, GaBr and GaI for ground state

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Keywords: GaF; GaCl; GaBr and GaI; vibrational-rotational energy; P(J); R(J)

ABSTRACT

A theoretical study of four gallium monohalides molecules (GaF, GaCl, GaBr and GaI) of ground state \( \Sigma^+ \) by using computer model is presented to study the energy characteristics of vibrational-rotational levels as a function of the vibrational and rotational quantum number, respectively. The calculations has been performed to examine the vibrational-rotational characteristics of some gallium halides molecules. These calculations appeared that all energies (\( G_v \), \( E_{vJ} \), and \( F_{vJ} \)) increase with increasing vibrational and rotational quantum number and by increasing the vibrational quantum number, and by increasing the vibrational quantum number, the vibrational constant will decrease. Also theoretical study of spectra of these molecules for ground state \( \Sigma^+ \) has been carried out. The values of spectral lines R(J) and P(J) were calculated and the relationship between the spectral lines and the rotational quantum number was established. The results appeared the spectra line values R(J) increases when the values of rotational quantum number decrease but the spectra line values P(J) decrease when the values of rotational quantum number increase, also the spectra line values P(J) decrease when the values of (m) increase, while the values of R(J) increase at first, then decrease showing Forrar parabola.

1. INTRODUCTION

The gallium monohalides play an important role as intermediates in the production of new high frequency and opto-electronic semiconductor devises[1]. Spectroscopic investigations on the diatomic halides of gallium have been the subject of much interest for a long time[2,3]. The general behavior of the spectrum of gallium monohalides is very similar to the one described for indium monohalides[4]. The ground state of all gallium monohalides is of the \( \Sigma^+ \) similar to other diatomic molecules formed by IIIA group elements (e.g., B, Al, Ga, and In) with halogens (e.g., F, Cl, Br, and I).

In 1933, Partrikaln and Hochberg[2] first observed the electronic spectrum of the GaCl radical. Miescher and Wehrli [5] recorded the electronic band spectrum of GaCl, GaBr, and GaI in both emission and absorption. Grabandt et al.[6] investigated the photoelectron spectra of gallium monohalide molecules. First measurements of pure rotational transitions of gallium monohalides GaCl, GaBr, and GaI were done by Barrett and Mendel[7].

Recently ab initio based MRDCI calculations on GaI molecule reported by Dutta et al.[8]. Further microwave spectral studies on the gallium monohalides have been carried out by a number of researchers and most recently, Lenthe et al.[9] performed DFT calculations to evaluate nuclear quadrupole coupling constants of a number of metal halide molecules, including the GaX molecules and most recently ab initio study of the ground state of GaCl reported by Yanget al.[10] also reveal that the ground states of GaI and GaCl are \( \Sigma^+ \) type.
2. THEORY

Theory of any vibrational–rotational state expressed in its wave number equivalent and measured in cm\(^{-1}\) units, can be written to a good approximation as[11]:

\[
E_{v',J} = G_v + B_v(J + 1) - D_vJ(J + 1)^2 + \cdots \cdots \cdot (1)
\]

Where \(v\): the vibrational quantum number equal 0,1,2,3,…etc., \(J\): the rotational quantum number equal 0,1,2,3,…etc., \(B_v\): rotational constant for vibrational state \(v\), \(D_v\): the centrifugal distortion constant for vibrational state \(v\), \(G_v\): the vibration energy.

The rotational energy is given by the following expression:

\[
F_{v,J} = J(J + 1)[B_v - \alpha_x (v + \frac{1}{2})] \cdots \cdots (4)
\]

Where: \(B_v\): the equilibrium rotational constant, \(\alpha_x\) the vibrational-rotational coupling constant, \(\omega_e\) the fundamental vibrational constant, \(\omega_{e\chi}\) the first anharmonic correction constant.

By satisfying the selection rules of vibrational quantum number \((\Delta v = 1)\) and rotational quantum number \((\Delta J = \pm 1)\), we have an allowed vibration-rotation absorption transition in diatomic will all electrons spin-paired. Those transition with \((\Delta J = -1)\) are said to be members of the " P branch" and those with \((\Delta J = +1)\) rome the " R branch".

The spectra lines were calculated using of the following equations[12]:

\[
R(J) = G_v + 2B_v(J + 1)(3B_{v'} - B_{v''})J + (B_{v'} - B_{v''})J^2 \quad (5)
\]

\[
P(J) = G_v - (B_{v'} + B_{v''})J + (B_{v'} - B_{v''})J^2 \quad (6)
\]

The Fortrat parabola curve could be found from the relation among \(R(J)\), \(P(J)\) and \(m\) using the following equation[13,14]:

\[
R(J), P(J) = G_v + (B_{v'} + B_{v''})m + (B_{v'} - B_{v''})m^2 \quad (7)
\]

By using equation (2), \(B_v\) rotational constant for vibrational state for all gallium halides is calculated and figure (1) and table (2) show its variation with the vibrational quantum number \(v\).

3. RESULTS AND DISCUSSION

In the present work, the calculations of the vibrational and rotational energy as a function of vibrational and rotational quantum number , respectively for gallium monohalides molecules (GaF, GaCl, GaBr and GaI) are presented by using computer model and by depended on spectroscopic constants for ground state \(\chi_{1\Sigma^+}^1\) for these molecules as shown in table (1).

| molecule | Spectroscopic constants of ground state \(\chi_{1\Sigma^+}^1\) in cm\(^{-1}\) and \(r_e\) in a.u.[15,6,9,16] |
|----------|--------------------------------------------------|
| GaF      | \(T_e\) | \(\omega_e\) | \(\omega_{e\chi}\) | \(r_e\) | \(B_e\) | \(\alpha_x\) |
|          | 0      | 622.10     | 3.286       | 1.774  | 0.359535 | 0.2864235 |
| GaCl     | 0      | 365.70     | 1.249       | 2.202  | 0.149913 | 7.9359    |
| GaBr     | 0      | 266.70     | 0.83        | 2.349  | 0.082797 | 3.26677   |
| GaI      | 0      | 216.60     | 0.50        | 2.576  | 0.056895 | 1.8890    |

By using equation (2), \(B_v\) rotational constant for vibrational state for all gallium halides is calculated and figure (1) and table (2) show its variation with the vibrational quantum number \(v\).
Table 2. Rotational constant in cm$^{-1}$ for vibrational state (\(v=1,2,\ldots,10\))

| V  | GaF   | GaCl   | GaBr   | GaI   |
|----|-------|--------|--------|-------|
| 0  | 0.3581| 0.1495 | 0.0828 | 0.0568|
| 1  | 0.3552| 0.1487 | 0.0825 | 0.0566|
| 2  | 0.3523| 0.1479 | 0.0822 | 0.0564|
| 3  | 0.3495| 0.1471 | 0.0819 | 0.0562|
| 4  | 0.3466| 0.1463 | 0.0816 | 0.0560|
| 5  | 0.3437| 0.1455 | 0.0813 | 0.0558|
| 6  | 0.3409| 0.1447 | 0.0810 | 0.0556|
| 7  | 0.338 | 0.1443 | 0.0807 | 0.0554|
| 8  | 0.3351| 0.1443 | 0.0804 | 0.0553|
| 9  | 0.3323| 0.1442 | 0.0801 | 0.0552|
| 10 | 0.3294| 0.1441 | 0.0798 | 0.0550|

It is seen that \(B_v\) decreases with increasing \(v\) for all molecules and particularly at high values of \(v\) for GaF. The values for GaCl, GaBr and GaI appear closest values that due to the small difference between the equilibrium rotational constant of these molecules.

The calculations of the vibrational energy of all molecules are made by using equation (3) and the results of calculation are shown in table (3) and figure (2). It can be seen that this factor varies linearly with the vibrational quantum number and the highest value is determined for GaF molecule, that is due to the fact the constants of the GaF molecule are several orders of magnitude larger than that for the other molecules (GaCl, GaBr and GaI).
Table 3. Vibration energy in cm\(^{-1}\) for vibrational state (v=1,2,…..10)

| V | GaF  | GaCl | GaBr | GaI  |
|---|------|------|------|------|
| 0 | 310.39 | 182.58 | 133.17 | 108.19 |
| 1 | 925.92 | 545.75 | 398.43 | 323.79 |
| 2 | 1534.88 | 906.43 | 662.23 | 538.39 |
| 3 | 2137.27 | 1264.61 | 924.57 | 751.99 |
| 4 | 2733.08 | 1620.29 | 1185.45 | 964.59 |
| 5 | 3327.33 | 1973.47 | 1444.88 | 1176.19 |
| 6 | 3904.99 | 2324.16 | 1702.86 | 1386.79 |
| 7 | 4481.09 | 2672.35 | 1959.38 | 1596.39 |
| 8 | 5050.63 | 3018.04 | 2214.44 | 1804.99 |
| 9 | 5613.58 | 3361.24 | 2468.04 | 2012.59 |
| 10 | 6169.97 | 3701.94 | 2720.19 | 2210.33 |

It is quite important to know the rotational energy levels \(F_{v,J}\) in order to predict the population of each vibrational-rotational level. Since the distribution of these level depends on the fraction of energy transferred to the vibrational degree of freedom of a molecule, which is a reaction product. By using the values of \(B_v\) to calculate the rotational energy (equation 4) as a function of the rotational quantum number at various values of vibrational quantum number \((v)\). the results of the rotational energy at vibrational states are presented in figures( 3,4,5,6and 7) and tables (4,5,6,7 and 8).

Table 4. Rotational energy in cm\(^{-1}\) at vibrational state (v=0) and J=(0,…10)

| J | GaF  | GaCl | GaBr | GaI  |
|---|------|------|------|------|
| 0 | 0    | 0    | 0    | 0    |
| 1 | 0.716 | 0.299 | 0.1656 | 0.1136 |
| 2 | 2.1486 | 0.897 | 0.4968 | 0.3408 |
| 3 | 4.2972 | 1.794 | 0.9936 | 0.6816 |
| 4 | 7.162 | 2.99 | 1.656 | 1.136 |
| 5 | 10.743 | 4.485 | 2.484 | 1.704 |
| 6 | 15.0402 | 6.279 | 3.4776 | 2.3856 |
| 7 | 20.0536 | 8.372 | 4.6368 | 3.1808 |
| 8 | 25.7832 | 10.764 | 5.9616 | 4.0896 |
| 9 | 32.229 | 13.455 | 7.452 | 5.112 |
| 10 | 39.391 | 16.445 | 9.108 | 6.248 |
Table 5. Rotational energy in cm\(^{-1}\) at vibrational state (v=1) and J=(0,…,10)

| J  | GaF  | GaCl  | GaBr  | GaI  |
|----|------|-------|-------|------|
| 0  | 0    | 0     | 0     | 0    |
| 1  | 0.7104 | 0.2974 | 0.165 | 0.11332 |
| 2  | 2.1312 | 0.8922 | 0.495 | 0.3396 |
| 3  | 4.2624 | 1.7844 | 0.99  | 0.6792 |
| 4  | 7.104  | 2.974  | 1.65  | 1.132 |
| 5  | 10.656 | 4.461  | 2.475 | 1.698 |
| 6  | 14.9184 | 6.2454 | 3.465 | 2.3772 |
| 7  | 19.8912 | 8.3272 | 4.62  | 3.1696 |
| 8  | 25.5744 | 10.7064 | 5.94  | 4.0752 |
| 9  | 31.968 | 13.383 | 7.425 | 5.094 |
| 10 | 39.072 | 16.357 | 9.075 | 6.226 |

Fig. (3) Rotational energy at vibrational state \(v=0\) as a function of rotational quantum number.
Table 6. Rotational energy in cm$^{-1}$ at vibrational state ($v=2$) and $J=(0,…,10)$

| J | GaF  | GaCl | GaBr | GaI  |
|---|------|------|------|------|
| 0 | 0    | 0    | 0    | 0    |
| 1 | 0.7046 | 0.2994 | 0.1644 | 0.1128 |
| 2 | 2.1138 | 0.8982 | 0.4932 | 0.3384 |
| 3 | 4.2276 | 1.7964 | 0.9864 | 0.6768 |
| 4 | 7.046  | 2.994  | 0.644  | 1.128  |
| 5 | 10.569 | 4.491  | 2.466  | 1.692  |
| 6 | 14.7966 | 6.2874 | 3.4524 | 2.3688 |
| 7 | 19.7288 | 8.3832 | 4.6032 | 3.1584 |
| 8 | 25.3656 | 10.7784 | 5.9184 | 4.0608 |
| 9 | 31.707 | 13.473 | 7.398 | 5.076 |
| 10| 38.753 | 16.467 | 9.042 | 6.204 |

Fig. (4) Rotational energy at vibrational state $v=1$ as a function rotational quantum number

Fig. (5) Rotational energy at vibrational state $v=2$ as a function rotational quantum number
Table 7. Rotational energy in cm\(^{-1}\) at vibrational state \((v=3)\) and \(J=(0,...,10)\)

| J  | GaF   | GaCl   | GaBr   | GaI   |
|----|-------|--------|--------|-------|
| 0  | 0     | 0      | 0      | 0     |
| 1  | 0.699 | 0.2834 | 0.1638 | 0.1124|
| 2  | 2.097 | 0.8502 | 0.4914 | 0.3372|
| 3  | 4.194 | 1.7004 | 0.9828 | 0.6744|
| 4  | 6.99  | 2.834  | 1.638  | 1.124 |
| 5  | 11.385| 4.251  | 2.457  | 1.686 |
| 6  | 15.939| 5.9514 | 3.4398 | 2.3604|
| 7  | 21.252| 7.9352 | 4.5864 | 3.1422|
| 8  | 27.324| 10.2024| 5.8968 | 4.0464|
| 9  | 34.155| 12.753 | 7.371  | 5.058 |
| 10 | 41.745| 15.587 | 9.009  | 6.182 |

**Fig. (6) Rotational energy at vibrational state \(v=3\) as a function rotational quantum number**
Table 8. Rotational energy in cm$^{-1}$ at vibrational state (v=4) and J=(0,…,10)

| J  | GaF   | GaCl  | GaBr  | GaI   |
|----|-------|-------|-------|-------|
| 0  | 0.6932| 0.2926| 0.1632| 0.112 |
| 1  | 2.0796| 0.8778| 0.4896| 0.336 |
| 2  | 4.1592| 1.7556| 0.9792| 0.672 |
| 3  | 6.9322| 2.926 | 1.632 | 1.12  |
| 4  | 10.3982| 4.389 | 2.448 | 1.68  |
| 5  | 14.5572| 6.1446| 3.4272| 2.352 |
| 6  | 19.4062| 8.1928| 4.5696| 3.136 |
| 7  | 24.9552| 10.5336| 5.8752| 4.032 |
| 8  | 31.1942| 13.167| 7.344 | 5.04  |
| 9  | 38.1262| 16.093| 8.976 | 6.16  |

From results above it is seen that the rotational energy increases with the rotational quantum number at vibrational states for all galliumes halides molecules and the highest value is determined for GaF at vibrational state v=3 as would be expected, and the lowest value is determined for GaI at vibrational state v=4. Also the values for GaCl, GaBr and GaI appear closet values that due to the small difference between the equilibrium rotational constant of these molecules, but values of GaF are far from values of other molecules by a small magnitudes that due to the difference in $B_e$ for GaF with other molecules is larger than the difference in $B_e$ between (GaCl, GaBr and GaI) molecules.

Also table (9) and figure (8) show the variation of the total energy which is called the vibrational-rotational energy at vibrational state v=0 as a function of rotational quantum number. it can be shown that the variation is as in figure (2) which means that the vibrational energy has predominate values in comparison with the rotational energy, all previous results are converge from other researchers values[17,18,19].
Table 9. Vibrational-rotational energy in cm\(^{-1}\) for vibrational state (v=0)

| J | GaF     | GaCl     | GaBr     | GaI     |
|---|---------|----------|----------|---------|
| 0 | 310.3863| 182.5828 | 133.173  | 108.1873|
| 1 | 311.1025| 182.8817 | 133.3385 | 108.3036|
| 2 | 312.5349| 183.4797 | 134.1665 | 108.8688|
| 3 | 314.6835| 184.3767 | 134.8289 | 109.528 |
| 4 | 317.5483| 185.5727 | 136.6505 | 110.2433|
| 5 | 321.1292| 187.0677 | 137.8097 | 111.3132|
| 6 | 325.4264| 188.8617 | 139.1345 | 112.1125|
| 7 | 330.4397| 190.9547 | 139.1345 | 113.4412|
| 8 | 336.1692| 193.3467 | 140.6249 | 114.352 |
| 9 | 342.6149| 196.0377 | 140.6249 | 114.352 |
| 10| 349.7768| 199.0276 | 142.2809 | 114.352 |

Fig. (8) Vibrational-rotational energy as a function of rotational quantum number at v=0

After that the spectra lines R(J) and P(J) values have been calculated for gallium halides molecules (GaF, GaCl, GaBr, and GaI) and (1-0) band by using equations (5 and 6), and by depended on spectroscopic constants in table (1). It appears from tables (10,11,12 and 13) and figures (9,10,11 and 12), that the spectral lines values R(J) and P(J) are influenced by difference between B\(_v\)' and B\(_\nu\)' . the spectral lines values R(J) increase with the increasing of J, whereas the spectra lines values P(J) decrease with the increasing of J. In addition note that the spectra line Q(J) was missing because in the \( \Sigma \) transition of the electronic angular moment A=0.
### Table 10. Spectra lines $P(J)$ and $R(J)$ in cm$^{-1}$ for (1-0) band of GaF molecule

For GaF molecule

| J | $P(J)$   | $R(J)$   |
|---|----------|----------|
| 0 | 615.532  | 616.2425 |
| 1 | 614.8158 | 616.9472 |
| 2 | 614.0939 | 617.6463 |
| 3 | 613.3662 | 618.3396 |
| 4 | 612.6329 | 619.0272 |
| 5 | 611.8938 | 619.7091 |
| 6 | 611.1512 | 620.3852 |
| 7 | 610.3985 | 621.0557 |
| 8 | 609.6422 | 621.7204 |
| 9 | 608.8803 | 622.6654 |
| 10| 608.1126 | 623.0327 |

![Graph showing the relation between spectra lines $R(J)$ and $P(J)$, measured in cm$^{-1}$ and rotational quantum number $J$ in the (1-0) band of GaF.](attachment:graph.png)
Table 11. Spectra lines $P(J)$ and $R(J)$ in cm$^{-1}$ for (1-0) band of GaCl molecule

| $J$ | $P(J)$   | $R(J)$   |
|-----|---------|---------|
| 0   | 363.1723| 363.4697|
| 1   | 362.8733| 363.7655|
| 2   | 362.5727| 364.0597|
| 3   | 362.2705| 364.3523|
| 4   | 361.9667| 364.6433|
| 5   | 361.6613| 364.9327|
| 6   | 361.3543| 365.2205|
| 7   | 361.0457| 365.5067|
| 8   | 360.7355| 365.7913|
| 9   | 360.4237| 366.0743|
| 10  | 360.1103| 366.3557|

Fig. (10) Relation between spectra lines $R(J)$ and $P(J)$ measured in cm$^{-1}$ and rotational quantum number $J$ in (1-0) band of GaCl

Table 12. Spectra lines $P(J)$ and $R(J)$ in cm$^{-1}$ for (1-0) band of GaBr molecule

| $J$ | $P(J)$   | $R(J)$   |
|-----|---------|---------|
| 0   | 265.254 | 265.419 |
| 1   | 265.0884| 265.5834|
| 2   | 264.9222| 265.7472|
| 3   | 264.7554| 265.9104|
| 4   | 264.588 | 266.073 |
| 5   | 264.42  | 266.235 |
| 6   | 264.2514| 266.3964|
| 7   | 264.0822| 266.5572|
| 8   | 263.9124| 266.7174|
| 9   | 263.742 | 266.876 |
| 10  | 263.571 | 267.036 |
Table 13. Spectra lines P(J) and R(J) in cm$^{-1}$ for (1-0) band of GaI molecule

| J  | P(J)   | R(J)   |
|----|-------|-------|
| 0  | 215.5992 | 215.7127 |
| 1  | 215.4853 | 215.8258 |
| 2  | 215.371  | 215.9385 |
| 3  | 215.2563 | 216.0508 |
| 4  | 215.1412 | 216.1627 |
| 5  | 215.0257 | 216.2742 |
| 6  | 214.9098 | 216.3853 |
| 7  | 214.7935 | 216.496  |
| 8  | 214.6768 | 216.6063 |
| 9  | 214.5597 | 216.7162 |
| 10 | 214.4422 | 216.8257 |
Equation (7) has been used to calculating Fortrat parabola and the results appear in tables (14,15,16 and 17) and figures (13,14,15 and 16). It appears that the spectra lines values R(J) at \( m = J + 1 \) increase at first, then decrease because the third term in right side of equation (7) becomes larger than the second one, therefore, we find that R(J) values deviate, forming Fortrat parabola and extreme curving representing the band head towards red region. As regards the spectra lines values P(J) at \( m = J \), they decrease when increasing \( m \) values.

Table 14. Spectra lines P(J) and R(J) in cm\(^{-1}\) for \((1-0)\) band of GaF molecule at \((J=0, 10, 20, 30, \ldots, 200)\)

| J  | P(J)  | R(J)  |
|----|-------|-------|
| 0  | 615.532 | 616.2425 |
| 10 | 616.2425 | 623.0327 |
| 20 | 629.2509 | 635.8752 |
| 30 | 639.9713 | 659.7479 |
| 40 | 644.4735 | 659.7924 |
| 50 | 654.4037 | 659.8391 |
| 60 | 651.7619 | 659.8991 |
| 70 | 654.5481 | 659.9405 |
| 80 | 658.7623 | 659.9933 |
| 90 | 658.4045 | 659.5253 |
| 100| 659.7479 | 658.0355 |
| 110| 659.7924 | 658.2457 |
| 120| 659.8391 | 653.8839 |
| 130| 659.8991 | 650.9501 |
| 140| 659.9405 | 647.4443 |
| 150| 659.9933 | 643.3665 |
| 160| 658.7623 | 643.3665 |
| 170| 658.4045 | 643.3665 |
| 180| 659.7479 | 643.3665 |
| 190| 659.7924 | 643.3665 |
| 200| 659.8391 | 643.3665 |

Fig. (13) Fortrat Parabola by \((1-0)\) band of GaF
Table 15. Spectra lines P(J) and R(J) in cm$^{-1}$ for (1-0) band of GaCl molecule at (J=0, 10, 20, 30, ……, 200)

| J   | m  | P(J)   | R(J)   |
|-----|----|--------|--------|
| 0   | 0  | 363.1723 | 1      | 363.7697 |
| 10  | -10| 360.1103 | 11     | 366.3557 |
| 20  | -20| 356.8883 | 21     | 369.0817 |
| 30  | -30| 353.5063 | 31     | 371.6477 |
| 40  | -40| 349.9643 | 41     | 374.0537 |
| 50  | -50| 346.2623 | 51     | 376.2997 |
| 60  | 61 | 378.3857 |        |          |
| 70  | 71 | 380.3117 |        |          |
| 80  | 81 | 382.0777 |        |          |
| 90  | 91 | 383.6837 |        |          |
| 100 | 101| 385.1297|        |          |
| 110 | 111| 386.4157|        |          |
| 120 | 121| 387.5417|        |          |
| 130 | 131| 388.5077|        |          |
| 140 | 141| 389.3137|        |          |
| 150 | 151| 389.9597|        |          |
| 160 | 161| 390.4457|        |          |
| 170 | 171| 390.7717|        |          |
| 180 | 181| 390.9377|        |          |
| 190 | 191| 390.9437|        |          |
| 200 | 201| 390.7897|        |          |

Fig. (14) Parabola by (1-0) band of GaCl
Table 16. Spectra lines $P(J)$ and $R(J)$ in cm$^{-1}$ for (1-0) band of GaBr molecule at 
(J=0, 10, 20, 30, ..., 200)

| J   | $P(J)$  | J   | $R(J)$  |
|-----|---------|-----|---------|
| 0   | 0       | 1   | 265.419 |
| 10  | -10     | 11  | 267.036 |
| 20  | -20     | 21  | 268.593 |
| 30  | -30     | 31  | 270.087 |
| 40  | -40     | 41  | 271.527 |
| 50  | -50     | 51  | 272.904 |
| 60  |         | 61  | 274.221 |
| 70  |         | 71  | 275.478 |
| 80  |         | 81  | 276.675 |
| 90  |         | 91  | 277.812 |
| 100 |         | 101 | 278.889 |
| 110 |         | 111 | 279.906 |
| 120 |         | 121 | 280.863 |
| 130 |         | 131 | 281.76  |
| 140 |         | 141 | 282.597 |
| 150 |         | 151 | 283.374 |
| 160 |         | 161 | 284.091 |
| 170 |         | 171 | 284.748 |
| 180 |         | 181 | 285.345 |
| 190 |         | 191 | 285.882 |
| 200 |         | 201 | 286.359 |

Fig. (15) Fortrat Parabola by (1-0) band of GaBr
Table 17. Spectra lines $P(J)$ and $R(J)$ in cm$^{-1}$ for $(1-0)$ band of GaI molecule at $(J=0, 10, 20, 30, \ldots, 200)$

| J   | For GaI molecule |
|-----|-----------------|
| 0   | $m$ | 0  | 215.5992 | 1  | 215.7127 |
| 10  | $m$ | -10 | 214.4422 | 11 | 216.8257 |
| 20  | $m$ | -20 | 213.2452 | 21 | 217.8987 |
| 30  | $m$ | -30 | 212.0082 | 31 | 218.9317 |
| 40  | $m$ | -40 | 210.7312 | 41 | 219.9247 |
| 50  | $m$ | -50 | 209.4142 | 51 | 220.8777 |
| 60  | $m$ |   61 | 221.7907 |   |   |
| 70  | $m$ |   71 | 222.6637 |   |   |
| 80  | $m$ |   81 | 223.4967 |   |   |
| 90  | $m$ |   91 | 224.2897 |   |   |
| 100 | $m$ | 101 | 225.0427 |   |   |
| 110 | $m$ | 111 | 225.7557 |   |   |
| 120 | $m$ | 121 | 226.4287 |   |   |
| 130 | $m$ | 131 | 227.0617 |   |   |
| 140 | $m$ | 141 | 227.6547 |   |   |
| 150 | $m$ | 151 | 228.2077 |   |   |
| 160 | $m$ | 161 | 228.7207 |   |   |
| 170 | $m$ | 171 | 229.1937 |   |   |
| 180 | $m$ | 181 | 229.6267 |   |   |
| 190 | $m$ | 191 | 230.0197 |   |   |
| 200 | $m$ | 201 | 230.3727 |   |   |

4. CONCLUSIONS

The main conclusion from this work that there is a small variation in the $G_v$, $E_{v,J}$, and $F_{v,J}$ for gallium monohalides molecules for different values of $v$ as it can be shown in all figures and the variation approximately in the same manners for all molecules except GaF molecule which has values far rather than other molecules, that due to rotational constant $B_v$ for this molecule. All
energies increase with increasing vibrational and rotational quantum number and by increasing the vibrational quantum number, the vibrational constant will decrease. The spectra line values $R(J)$ increases when the values of rotational quantum number decrease but the spectra line values $P(J)$ decrease when the values of rotational quantum number increase. Also the spectra line values $P(J)$ were decrease when the values of $(m)$ increase, while the values of $R(J)$ increase at first, then decrease showing Fortrar parabola.

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( Received 07 April 2015; accepted 22 April 2015 )