



Research article

Analytical solutions and Herzberg's energy level for modified shifted morse molecular system

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ABSTRACT

The solution of the radial Schrödinger equation for the modified shifted Morse potential model is obtained using an approximate supersymmetric approach. The two different formulae for the computation of the centrifugal distortion constant are clearly examined to deduce the formula that gives the result that perfectly aligns with the experimental data. Numerical values for different molecules are computed for the two different values of the centrifugal distortion constant (dissociation energy) obtained from two different equations. The ground state energy spectra for different molecules are obtained using Herzberg's energy level equation as a standard for some molecules. The results of the modified shifted Morse potential are compared with the results from Herzberg's energy level equation and the experimental data. Our study reveals that the results for one of the two centrifugal distortion constants are closer to the standard results and the experimental data in all the molecules studied.

1. Introduction

The accurate solution of the Schrödinger equation for electronic motion is possible for simple cases [1], hence the derivation of $U(r)$ curves by other means is necessary. The accurate potential energy curves of diatomic molecules is essentially required to evaluate the Franck-Condon factors for transitions between their various electronic states. According to Coxon [2], the possibility of the variation of the potential energy with r by approximate analytical function can be evaluated. The representation can only be done by system like Morse potential model for spectroscopic data that are limited to a few low-lying levels of an electronic state. The spectroscopic constants of the molecules such as diatomic molecules, can be predicted with a fairly good accuracy. This can be achieved by fitting their potential energy curves from the electronic states [3]. Hence, the production of spectra solemnly depends upon the correctness of the spectroscopic constants employed as a standard. These standards validate new theoretical methods like electron correlation, quality of new basis, and others.

Over the years, different authors have reported the solutions of the Schrödinger equation in terms of bound state and energy spectra for both central and non-central physical potential models [4-6] using different traditional techniques. The choice of each technique

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depends on its simplicity, author's understanding and its application to the problem. Recently, interest have been devoted to the description of theoretical fitness of some molecules for different physical potential energy function. For instance, the eigenvalues of cesium dimer was reported under the improved Manning-Rosen and Tietz-Hua potential energy models [7]. The calculated results for the two potential models strongly aligned with the observed data. The spectra for 6^1I_u state of lithium dimer and $X^3 \text{I}$ state of silicon carbide were studied under the improved Rosen-Morse potential model [8]. In Ref. [9], the authors studied some molecules under the improved Pöschl-Teller potential model. Jia et al. [10] in one of their papers, studied CP molecule under the improved Tietz potential function. The calculated results agreed with the experimental data. Recently, Onate et al. [11], studied chlorine molecule under the molecular attractive potential model. Their calculated results perfectly agreed with the ground state energy computed by Coxon using Herzberg' energy level. However, several reports have predicted various spectroscopic constants with high degree of accuracy to determine the spectra of different molecules in the non-relativistic regime. Such constants include the B_e , the harmonic vibrational frequency ω_e , the vibrational anharmonicity $\omega_e x_e$, the equilibrium bond length r_e , the centrifugal distortion constant D_e and the vibration-rotation interaction constant α_e . The accurate analytical determination of spectra for different molecules, depends on the correctness of the values of the spectroscopic constants used. A clear understanding of the spectroscopic study revealed that the spectroscopic constants were experimentally deduced for theoretical application. In the theoretical analysis, it has been revealed that the centrifugal distortion constant can be calculated from other spectroscopic constants for cases where its value in the experimental deduction is not given. A deep study shows from the literature that there are two different equations for the theoretical computation of the centrifugal distortion constant. Our interaction with the two equations provided different results. The two different equations are given as [12,13]

$$D_e^1 = \omega_e^2 / 4\omega_e x_e, \quad (1)$$

$$D_e^2 = \omega_e^2 / (5.33\omega_e x_e - 2B_e). \quad (2)$$

The variation in the result for the centrifugal distortion constant raises an issue as to which of the equation gives the value of the centrifugal distortion constant that will fit a molecular description when compared with experimental data. Hence, the necessity for this study since the analytical spectra for molecules depends on the spectroscopic constants that includes the centrifugal distortion constant. Motivated by theoretical determination of molecular spectra in the non-relativistic domain, the present study aims to determine equation that gives the value of the centrifugal distortion constant that aligned the theoretical values with experimental data perfectly. The objectives of this study are as follows.

- (i). to calculate the energy equation for modified shifted Morse potential via supersymmetric approach.
- (ii) to calculate the centrifugal distortion constant using Eq. (1) and Eq. (2) respectively.
- (iii) to compute numerical results for some molecules using the results of Eq. (1) and Eq. (2) and compare the calculated results with the experimental data.
- (iv) to calculate the ground state energy level using Herzberg's energy level equation as a standard for molecules that we cannot access the experimental data.

The modified shifted Morse potential model is given as [14]

$$V(r) = D_e [(\ell + \beta)^2 - (2\ell + 3\gamma)e^{-\alpha(r-r_e)} + e^{-2\alpha(r-r_e)}] \quad (3)$$

where ℓ , γ and β are potential parameters, r_e is the bond separation and r is the inter-nuclear separation. By employing the conditions to be satisfied by diatomic molecular potential function, the potential parameters are obtained as

$$\left. \begin{aligned} \frac{dV(r)}{dr} \Big|_{r=r_e} &= 0, \\ V(r \rightarrow \infty) - V(r_e) &= D_e, \\ \frac{d^2V(r)}{dr^2} \Big|_{r=r_e} &= 4\pi\mu c^2 \omega_e^2 \end{aligned} \right\} \quad (4)$$

where c is the speed of light. For the modified shifted Morse potential function to completely fit the description of the diatomic molecules, the following relations are established between the potential parameters

$$\left. \begin{aligned} 3\gamma + 2\ell &= 2 \\ \ell + \beta &= 1 \end{aligned} \right\} \quad (5)$$

When $\ell = 1$, β and γ respectively, must be zero. After some mathematical simplifications using the relations in Eq. (4), the parameter α for molecular system can be calculated by the formula

$$\alpha = 2\pi c \omega_e \sqrt{\frac{\mu}{D_e(4 - 2\ell - 3\gamma)}} \quad (6)$$

To compute the spectra for any molecule, the conditions given in Eq. (5) and Eq. (6) must be obeyed.

2. Bound state solutions

To obtain the non-relativistic solutions for any quantum system of a given physical potential model, the radial Schrödinger equation with an interacting potential $V(r)$ and non-relativistic energy $E_{v,j}$ is given as

$$\left(\frac{d^2}{dr^2} + \frac{2\mu E_{v,j}}{\hbar^2}\right)U_{v,j}(r) = \left(\frac{j(j+1)}{r^2} + \frac{2\mu V(r)}{\hbar^2}\right)U_{v,j}(r), \tag{7}$$

where μ is the reduced mass of the molecule, v is the vibrational quantum state, \hbar is the reduced Planck's constant and $U_{v,j}(r)$ is the radial wave function. To obtain the solutions of Eq. (7), the use of approximation scheme is recommended. It is noted that the following formula

$$\frac{1}{r^2} \approx \frac{d_0 + d_1 e^{-ar} + d_2 e^{-2ar}}{r_e^2}, \tag{8}$$

is suitable for the centrifugal term in Eq. (7), where

$$d_0 = 1 + \frac{3}{\alpha r_e} \left(\frac{1}{\alpha r_e} - 1\right), d_1 = \frac{2e^{ar_e}}{\alpha r_e} \left(2 - \frac{3}{\alpha r_e}\right), d_2 = \frac{e^{2ar_e}}{\alpha r_e} \left(\frac{3}{\alpha r_e} - 1\right) \tag{9}$$

Eq. (9) gives the values of the parameters in Eq. (8). Plugging Eq. (3) and Eq. (8) into Eq. (7) gives the following second-order differential equation

$$\frac{d^2 U_{v,j}(r)}{dr^2} = V_T U_{v,j}(r) + V_P e^{-ar} U_{v,j}(r) + V_R e^{-2ar} U_{v,j}(r) \tag{10}$$

where

$$\left. \begin{aligned} V_T &= \frac{Jd_0}{r_e^2} + \frac{2\mu(D_e(\ell + \beta)^2 - E_{v,j})}{\hbar^2}, \\ V_P &= \frac{Jd_1}{r_e^2} - \frac{2\mu D_e(2\ell + 3\gamma)e^{ar_e}}{\hbar^2}, \\ V_R &= \frac{Jd_2}{r_e^2} + \frac{2\mu D_e e^{2ar_e}}{\hbar^2}, \\ J &= j(j+1) \end{aligned} \right\} \tag{11}$$

The parameters in Eq. (11) are used for simplicity. Following the supersymmetric approach [15-17], the ground state wave function written in the form

$$U_{0,j}(r) = \exp\left(-\int W(r)dr\right) \tag{12}$$

corresponding to the two partner Hamiltonians

$$\left. \begin{aligned} H_- &= \widehat{A}^\dagger \widehat{A} = -\frac{d^2}{dr^2} + V_-(r), \\ H_+ &= \widehat{A} \widehat{A}^\dagger = -\frac{d^2}{dr^2} + V_+(r) \end{aligned} \right\} \tag{13}$$

where

$$\left. \begin{aligned} \widehat{A} &= \frac{d}{dr} - W(r), \\ \widehat{A}^\dagger &= -\frac{d}{dr} - W(r), \\ V_\pm(r) &= W^2(r) \pm \frac{dW(r)}{dr} \end{aligned} \right\} \tag{14}$$

where the Hamiltonians in Eq. (13) are clearly defined in Eq. (14) and $W(r)$ is called superpotential function is supersymmetry quantum mechanics. Plugging Eq. (12) into Eq. (10) gives a nonlinear Riccati equation of the form

$$W^2(r) - \frac{dW(r)}{dr} = \frac{J(d_0 + d_1 + d_2)}{r_e^2} + \frac{2\mu(D_e(\ell + \beta)^2 - E_{0,j})}{\hbar^2} - \frac{2\mu D_e(2\ell + 3\gamma)e^{ar_e}}{\hbar^2} + \frac{2\mu D_e e^{2ar_e}}{\hbar^2}, \tag{15}$$

whose solution can only be obtained by proposing a superpotential function of the form

$$W(r) = \rho_0 - \frac{\rho_1}{e^{ar}}. \tag{16}$$

The two parameters ρ_0 and ρ_1 are superpotential constants. Substituting Eq. (16) into Eq. (15) with the consideration that the radial wave equation satisfy the boundary conditions for $R_{n,\ell}(r)/r$ becomes zero as $r \rightarrow \infty$, and $R_{n,\ell}(r)/r$ is finite when $r = 0$, together with some mathematical manipulations and simplifications, the two superpotential constants in Eq. (16) can be obtain as

$$\rho_0^2 = -\frac{2\mu E_{v,j}}{\hbar^2} + \frac{2\mu D_e(\ell + \beta)^2}{\hbar^2} + \frac{Jd_0}{r_e^2}, \tag{17}$$

$$\rho_1 = \sqrt{\frac{Jd_2}{r_e^2} + \frac{2\mu D_e e^{2ar_e}}{\hbar^2}}, \tag{18}$$

$$\rho_0 = \frac{\frac{2\mu D_e(2\ell+3\gamma)e^{ar_e}}{\hbar^2} - \frac{Jd_1}{r_e^2} - \alpha\rho_1}{2\rho_1}. \tag{19}$$

Eq. (17), Eq. (18) and Eq. (19) stand for the superpotential constants. Comparing the partner Hamiltonians and Eq. (16), the two partner potentials in the supersymmetry quantum mechanics can be constructed as

$$V_+(r) = W^2(r) + \frac{dW(r)}{dr} = \rho_0^2 - \rho_1(2\rho_0 - \alpha)e^{-ar} + \rho_1^2 e^{-2ar}, \tag{20}$$

$$V_-(r) = W^2(r) - \frac{dW(r)}{dr} = \rho_0^2 - \rho_1(2\rho_0 + \alpha)e^{-ar} + \rho_1^2 e^{-2ar}. \tag{21}$$

It can be seen from Eq. (20) and Eq. (21) that the family potentials satisfied a shape invariance condition which established a relation of the form

$$V_+(a_0, r) = V_-(a_1, r) + R(a_1), \tag{22}$$

where a_1 is a new set of parameters uniquely determined from an old set of parameters a_0 , the term $R(a_1)$, is called a remainder or residual term that is independent of the variable r . The partner potentials revealed that the shape invariance holds after a mapping of the form $\rho_1 \rightarrow \rho_1 + \alpha$ [18,19]. From Eq. (22), it can easily be shown that

$$R(a_1) = \left(-\frac{V_P - a_0}{2a_0}\right)^2 - \left(-\frac{V_P - a_1}{2a_1}\right)^2, \tag{23}$$

$$R(a_2) = \left(-\frac{V_P - a_1}{2a_1}\right)^2 - \left(-\frac{V_P - a_2}{2a_2}\right)^2, \tag{24}$$

$$R(a_3) = \left(-\frac{V_P - a_2}{2a_2}\right)^2 - \left(-\frac{V_P - a_3}{2a_3}\right)^2, \tag{25}$$

and finally

$$R(a_n) = \left(-\frac{V_P - a_{n-1}}{2a_{n-1}}\right)^2 - \left(-\frac{V_P - a_n}{2a_n}\right)^2. \tag{26}$$

Using Eq. (23), Eq. (24), Eq. (25) and Eq. (26), the eigenvalues can now be deduce as

$$E_{v,j} = \sum_{k=1}^n R(a_k) = \left(-\frac{V_P - a_0}{2a_0}\right)^2 - \left(-\frac{V_P - a_n}{2a_n}\right)^2 \tag{27}$$

The final energy equation for the modified shifted Morse potential model in the non-relativistic regime can be obtained following Eq. (27)

$$E_{v,j} = D_e(\ell + \beta)^2 + \frac{Jd_0\alpha^2\hbar^2}{2\mu r_e^2} - \frac{\alpha^2\hbar^2}{2\mu} \left(\frac{\frac{\mu D_e(2\ell+3\gamma)e^{ar_e}}{\alpha^2\hbar^2} - \frac{Jd_1}{r_e^2} - \left(v + \frac{1}{2}\right)\sqrt{\frac{Jd_2}{\alpha^2 r_e^2} + \frac{2\mu D_e e^{2ar_e}}{\alpha^2\hbar^2}}}{\sqrt{\frac{Jd_2}{\alpha^2 r_e^2} + \frac{2\mu D_e e^{2ar_e}}{\alpha^2\hbar^2}}} \right)^2 \tag{28}$$

The corresponding un-normalized radial wave function is given as

$$R_{v,j}(y) = Ny \sqrt{\frac{2\mu D_e (\gamma + \beta)^2}{\alpha^2 \hbar^2} + Jd_0 - \frac{2\mu E_{v,j}}{\alpha^2 \hbar^2}} e^{-y} \sqrt{\frac{2\mu D_e e^{2\alpha r_e}}{\alpha^2 \hbar^2} + \frac{Jd_2}{\alpha^2 r_e^2}} L_n^2 \sqrt{\frac{2\mu D_e (\gamma + \beta)^2}{\alpha^2 \hbar^2} + Jd_0 - \frac{2\mu E_{v,j}}{\alpha^2 \hbar^2}} \left(2 \sqrt{\frac{2\mu D_e e^{2\alpha r_e}}{\alpha^2 \hbar^2} + \frac{Jd_2}{\alpha^2 r_e^2}} y \right). \quad (29)$$

Eq. (28) is the energy equation while Eq. (29) is the radial wave function.

2.1. Herzberg's energy level equation

Herzberg's energy level equation will be used to compute results for molecules whose experimental data are not available to us. The results will be taken as standard values. The Herzberg's energy level equation is given by [12,13,20].

$$G(v) = E(v) = \omega_e(v + 0.5) - \omega_e x_e(v + 0.5)^2, v = 0, 1, 2, \dots \quad (30)$$

where v is the vibrational quantum state. The details of how Eq. (30) is obtained is not given in this study but can be found in the literature.

3. Results

4. Discussion

The spectroscopic constants for the molecules studied in this work are presented in Table 1. In Tables 2-5, the results for ScF, P₂, IF and ICl molecules respectively are given. The results under $G(v)$ is the ground state energy obtained from Eq. (30). The values are taken as standard for molecules whose observed data can not be found. The results under D_e^1 are obtained with D_e deduced from Eq. (1) while those under D_e^2 are obtained with D_e from Eq. (2). The calculated results for the modified shifted Morse potential model with D_e from each of Eq. (1) and Eq. (2) strongly agreed with the ground state energy as standard ($G(v)$). To deduce the accuracy of the calculated results, the average absolute percentage deviation of the $G(v)$ results are obtained. In Table 2, the deviation for D_e^1 (using D_e in Eq. (1)) is 0.0000027% while that of D_e obtained in Eq. (2) has the percentage deviation as 0.1015% for ScF molecule. For P₂ molecule in Table 3, the average absolute percentage deviation are 0.00000164% and 0.0716% with the values of D_e in Eq. (1) and Eq. (2) respectively. In Table 4, it is 0.00000547% and 0.054% for IF. For ICl, it is 0.00000635% and 0.3086% in Table 5. The average absolute percentage deviation of the $G(v)$ values showed that the computed results for the modified shifted Morse potential perfectly fits the description of molecules. However, the results obtained with the centrifugal distortion constant in Eq. (1) are almost the same as the $G(v)$ results. It can be seen that the average absolute percentage deviation is almost zero. In Tables 6-8, the experimental (RKR) data and the calculated results for H₂, CO and HF respectively are presented. For each of D_e in Eq. (1) or Eq. (2) used, the calculated results perfectly aligned with the RKR data. The average absolute percentage deviation using D_e in Eq. (1) and Eq. (2) respectively are 0.0695% and 0.2470% for H₂ in Table 6. It is 0.0045% and 0.1178% for CO in Table 7 while in Table 8, it is 0.1554% and 0.5517% for HF. It is observed that the deviation of the calculated results from the $G(v)$ values and RKR data increase with increase in the vibrational quantum state. The results in all the Tables revealed that even when the calculated results strongly agreed with the RKR data and the $G(v)$ values, the results obtained with the value of centrifugal distortion in Eq. (1) are closer to the RKR values than the results obtained with the value of centrifugal distortion in Eq. (2). A clear observation shows that the average absolute percentage deviation for the RKR data with the two values of the centrifugal distortion constant are closer compared to the average absolute percentage deviation of the $G(v)$ values.

5. Conclusion

The solution for modified shifted Morse potential was obtained using supersymmetric approach. This study revealed that the modified shifted Morse potential model is a good representation for molecular description. The results obtained with two different values of the centrifugal distortion showed a strong agreement with both the RKR data and the results of $G(v)$. However, the results

Table 1
Molecules and their spectroscopic constants [21,22].

Molecule	$\omega_e(\text{cm}^{-1})$	$\omega_e x_e(\text{cm}^{-1})$	$B_e(\text{cm}^{-1})$	$r_e(\text{\AA})$
ScF($X^1\Sigma^+$)	717	3.7	0.396	1.7857
P ₂ ($X^1\Sigma_g^+$)	788	2.9	0.301	1.9017
IF($B^3\Pi(0)$)	406.51	1.30	0.2272	2.1189
ICl($B^3\Pi(0^+)$)	204.5	2.595	0.08705	2.657
IBr($B^3\Pi(0^+)$)	142	2.6	0.0432	2.83
H ₂ ($X^1\Sigma_g^+$)	4401.265	120.6020	60.8477	0.5039
CO($X^1\Sigma^+$)	2169.813	13.2883	1.9314	1.1283
HF($X^1\Sigma^+$)	4138.32	89.88	20.9557	0.9168

Table 2The comparison of the results (cm^{-1}) for two values of the centrifugal distortion constant (D_e) for ScF molecule.

ν	$G(\nu)$	D_e^1	D_e^2
0	357.5750	357.5750	357.3169
1	1067.1750	1067.1751	1064.8525
2	1769.3750	1769.3752	1762.9237
3	2464.1750	2464.1753	2451.5304
4	3151.5750	3151.5756	3130.6726
5	3831.5750	3831.5758	3800.3505
6	4504.1750	4504.1762	4460.5639
7	5169.3750	5169.3765	5111.3129
8	5827.1750	5827.1770	5752.5974
9	6477.5750	6477.5775	6384.4175
10	7120.5750	7120.5780	7006.7732
11	7756.1750	7756.1786	7619.6645
12	8384.3750	8384.3793	8223.0913
13	9005.1750	9005.1800	8817.0537
14	9618.5750	9618.5808	9401.5516
15	10224.5750	10224.5816	9976.5851

Table 3The comparison of the results (cm^{-1}) for two values of the centrifugal distortion constant (D_e) for P_2 molecule.

ν	$G(\nu)$	D_e^1	D_e^2
0	393.2750	393.2750	393.0716
1	1175.4750	1175.4750	1173.6440
2	1951.8750	1951.8751	1946.7889
3	2722.4750	2722.4752	2712.5062
4	3487.2750	3487.2754	3470.7960
5	4246.2750	4246.2756	4221.6582
6	4999.4750	4999.4758	4965.0928
7	5746.8750	5746.8761	5701.0999
8	6488.4750	6488.4763	6429.6794
9	7224.2750	7224.2767	7150.8314
10	7954.2750	7954.2771	7864.5558
11	8678.4750	8678.4775	8570.8526
12	9396.8750	9396.8779	9269.7219
13	10109.4750	10109.4784	9961.1636
14	10816.2750	10816.2789	10645.1778
15	11517.2750	11517.2795	11321.7644

Table 4The comparison of the results (cm^{-1}) for two values of the centrifugal distortion constant (D_e) for IF molecule.

ν	$G(\nu)$	D_e^1	D_e^2
0	202.9300	202.9300	202.8503
1	606.8400	606.8400	606.1231
2	1008.1500	1008.1500	1006.1585
3	1406.8600	1406.8600	1402.9566
4	1802.9700	1802.9701	1796.5175
5	2196.4800	2196.4801	2186.8411
6	2587.3900	2587.3901	2573.9274
7	2975.7000	2975.7002	2957.7764
8	3361.4100	3361.4102	3338.3881
9	3744.5200	3744.5203	3715.7626
10	4125.0300	4125.0304	4089.8997
11	4502.9400	4502.9404	4460.7996
12	4878.2500	4878.2505	4828.4622
13	5250.9600	5250.9606	5192.8875
14	5621.0700	5621.0707	5554.0756
15	5988.5800	5988.5808	5912.0263

obtained with the centrifugal distortion deduced from the formula $D_e^1 = \omega_e^2/4\omega_e x_e$, are closer to the $G(\nu)$ results and the RKR data compared to the results obtained with the centrifugal distortion with formula $D_e^2 = \omega_e^2/(5.33\omega_e x_e - 2B_e)$. This study also shows that the ground state energy obtained from Herzberg's energy level equation and the experimental data are never the same but very close. Finally, the centrifugal distortion constant in Eq. (1) is preferable for any computation because the value of D_e obtained from Eq. (1) for

Table 5The comparison of the results (cm^{-1}) for two values of the centrifugal distortion constant (D_e) for ICl molecule.

ν	$G(\nu)$	D_e^1	D_e^2
0	101.6012	101.6012	101.3964
1	300.9113	300.9112	299.0677
2	495.0313	495.0311	489.9104
3	683.9612	683.9610	673.9243
4	867.7012	867.7009	851.1095
5	1046.2513	1046.2507	1021.4661
6	1219.6112	1219.6105	1184.9940
7	1387.7813	1387.7803	1341.6932
8	1550.7613	1550.7600	1491.5637
9	1708.5513	1708.5497	1634.6055
10	1861.1512	1861.1494	1770.8186
11	2008.5613	2008.5591	1900.2030
12	2150.7813	2150.7787	2022.7588
13	2287.8112	2287.8082	2138.4858
14	2419.6512	2419.6478	2247.3842
15	2546.3013	2546.2973	2349.4539

Table 6The comparison of the experimental data and calculated results (cm^{-1}) for two values of the centrifugal distortion constant (D_e) for H_2 molecule.

ν	RKR [23]	D_e^1	D_e^2
0	2170.08	2170.4819	2168.0633
1	6331.22	6330.5424	6308.7745
2	10257.19	10249.3984	10188.9318
3	13952.43	13927.0499	13808.5354
4	17420.44	17363.4969	17167.5852
5	20662.00	20558.7394	20266.0811
6	23675.73	23512.7774	23104.0233
7	26457.91	26225.6109	25681.4116
8	29001.05	28697.2398	27998.2461
9	31294.01	30927.6643	30054.5268

Table 7The comparison of the experimental data and calculated results (cm^{-1}) for two values of the centrifugal distortion constant (D_e) for CO molecule.

ν	RKR [24]	D_e^1	D_e^2
0	1081.7791	1081.5844	1080.7213
1	3225.0522	3224.8208	3217.0523
2	5341.8437	5341.4806	5319.9015
3	7432.2200	7431.5638	7389.2687
4	9496.2494	9495.0704	9425.1540
5	11534.0013	11532.0004	11427.5574
6	13545.5470	13542.3538	13396.4789
7	15530.9592	15526.1306	15331.9185
8	17490.3124	17483.3308	17233.8761
9	19423.6825	19413.9544	19102.3518
10	21331.1469	21318.0014	20937.3456
11	23212.7846	23195.4718	22738.8575
12	25068.6758	25046.3655	24506.8874
13	26898.9019	26870.6827	26241.4354
14	28703.5456	28668.4233	27942.5015
15	30482.6901	30439.5873	29610.0857

different molecules gives a closer result to experimental data and $G(\nu)$ values.

Author contribution statement

C.A. Onate: Conceived and designed the analysis; Analysed and interpreted the data.

I.B. Okon: Analyzed and interpreted the data; Wrote the paper.

D.T. Bankole: Contributed analysis tools or data; Wrote the paper.

Table 8

The comparison of the experimental data and calculated results (cm^{-1}) for two values of the centrifugal distortion constant (D_e) for HF molecule.

ν	RKR [25]	D_e^1	D_e^2
0	2050.76	2046.6900	2041.8382
1	6012.18	6005.2500	5961.5837
2	9801.58	9784.0500	9662.7547
3	13423.56	13383.0900	13145.3512
4	16882.39	16802.3700	16409.3732
5	20181.72	20041.8899	19454.8207
6	23324.52	23101.6499	22281.6937
7	26313.03	25981.6499	24889.9922
8	29148.72	28681.8899	27279.7162
9	31832.11	31202.3698	29450.8657
10	34362.58	33543.0898	31403.4407
11	36738.08	35704.0497	33137.4412
12	38954.72	37685.2497	34652.8672
13	41006.39	39486.6897	35949.7187
14	42884.20	41108.3696	37027.9957
15	44575.74	42550.2895	37887.6981

G.O. Egharevba: Contributed analysis tools or data; Analysed and interpreted the data.

M.O. Oluwayemi: Analyzed and interpreted the data; Contributed the analysis tools or data.

J.A. Owolabi: Contributed analysis tools or data; Wrote the paper.

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Data availability statement

Data will be made available on request.

Declaration of interest's statement

The authors declare no competing interests.

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