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Ro-vibrating energy states of a diatomic molecule in an empirical potential

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Abstract An approximate analytical solution of the Schrödinger equation is obtained to represent the rotational–vibrational (ro-vibrating) motion of a diatomic molecule. The ro-vibrating energy states arise from a systematical solution of the Schrödinger equation for an empirical potential (EP) $V_{\pm}(r) = D_e\{1 - (\varepsilon/\delta)[coth\,(\eta r)]^{\pm 1}/1 - (\varepsilon/\delta)\}^2$ are determined by means of a mathematical method so-called the Nikiforov–Uvarov (NU). The effect of the potential parameters on the ro-vibrating energy states is discussed in several values of the vibrational and rotational quantum numbers. Moreover, the validity of the method is tested with previous models called the semiclassical (SC) procedure and the quantum mechanical (QM) method. The obtained results are applied to the molecules H_2 and Ar_2.

Keywords Diatomic molecule · Empirical potential · Ro-vibrating energy state · Nikiforov–Uvarov method

1 Introduction

The investigation of the rotational–vibrational motion of a diatomic molecule by means of the direct solution of the Schrödinger equation is beginning to make a major impact in the area of the experimental spectroscopy which is used to determine the spectroscopic parameters of diatomic molecules [1]. Spectroscopic techniques are fundamental in studying electronic structures, spectroscopic constants and energetic properties of diatomic molecules. Moreover, these techniques are also required for parametrization of new methods based on theoretical analysis and computational calculations [2]. In the theoretical and computational studies, the electronic and nuclear parts of

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the Schrödinger equation are solved separately via the Born-Oppenheimer approximation [3]. To obtain a representative sample of geometrical configurations of the nuclei, the electronic part is firstly solved in space and hence the relative positions of the nuclei are described by a function of the space coordinates. The Schrödinger equation is finally solved using this function called the Born-Oppenheimer potential energy surface. Although computational efforts have been directed to calculate potential energy surfaces for polyatomic molecules with spectroscopic accuracy [4], it is also appropriate to study the applicability of the algebraic approaches [5–20]. Most of these approaches have been applied to problems in molecular physics for a number of years to understand the rotational–vibrational dynamics of diatomic molecules [21]. In molecular physics, the most of the physical applications of quantum algebras have been used for describing rotation–vibration spectra of diatomic molecules [22–24]. A phenomenological model for vibrational–rotational spectroscopy of molecules has been compactly expressed using the quantum-group theoretic approach [25,26]. This model has been also applied to the description of rotational bands of various atomic nuclei [27–29].

The vibration of molecules is the best described using a quantum mechanical approach. Molecules do not behave according to a harmonic oscillator description used as an approximate treatment for low vibrational quantum numbers. On the contrary, the effect of bond breaking on the vibration of molecules is better explained by an exponential type of potential than the harmonic oscillator. This type of exponential potential is known the Morse potential [30] and it is a convenient model for the potential energy of a diatomic molecule. The Morse potential was introduced with the purpose of producing an accurate description of typical spectra of diatomic molecules through the analytically solvable Schrödinger equation. It is well-known that the Morse potential is still one of the few model potentials which allow an exact solution for the energy levels and wave functions, when it is used in the Schrödinger equation for a vibrating diatomic molecule in the case of $\ell\, l = 0$, where ℓ is the angular momentum quantum number. Moreover, the ro-vibrating motion of a diatomic molecule for any ℓ can be described by means of some analytical methods [31]. It is clear that the Morse potential has a finite value at $r = 0$ and, cannot satisfy the boundary conditions. In the region of large r, the theoretical value for the well depth of the Morse potential is smaller than the experimental one. In this region, a more suitable potential function should be suggested to remove the difference between the theory and experiment. To improve some inaccuracies of the Morse potential, an empirical potential (EP) function was suggested by Schiöberg [32]. The simple form of the EP is introduced as follows

$$V_{\pm}(r) = D\{\delta - \varepsilon\,[coth(\eta r)]^{\pm 1}\}^2, \tag{1}$$

where δ, ε and η are the setting parameters of the potential and $D = D_e/(\delta - \varepsilon)^2$ (D_e is the spectroscopic dissociation energy). The EP has a minimum value 0 at the point of $r = r_e$

$$r = r_e = \frac{1}{\eta}\, arctanh\left(\frac{\varepsilon}{\delta}\right)^{\pm 1}, \tag{2}$$

and approaches D_e exponentially for large r. The functional forms of the EP given in Eq. 1 are significant in the limits of $0 \leq \varepsilon < \delta$ for $V_+(r)$ and $\varepsilon < \delta \leq 0$ for $V_-(r)$ [32].

The solution of the Schrödinger equation for an empirical potential (EP) gives the ro-vibrating energy states of a diatomic molecule. This solution serves as the basis for the description of the quantum aspects of diatomic molecules. In the present study, for this reason, ro-vibrating energy states of a diatomic molecule in the EP is approximately calculated by means of the Nikiforov–Uvarov (NU) method [33]. The proposed method is advantageously applied to calculate the ro-vibrating energy states of the molecules H_2 and Ar_2. The method used in this study is an alternative to previous models called Semiclassical (SC) procedure and Quantum Mechanical (QM) method. For more information on the NU method, one can refer to the recent theoretical works [31,34–38] where the details of how to derive the energy states for a given potential have been presented by introducing the basic equations of the method.

2 Ro-vibrating energy states in the EP

After having separate the angle-dependent and radial parts of the Schrödinger equation for a diatomic molecule with the reduced mass μ, the relevant differential equation for the radial motion is described as

$$\left(\frac{d^2}{dr^2} - \frac{L}{r^2} + \frac{2\mu}{\hbar^2}(E - V_\pm(r))\right) R(r) = 0, \tag{3}$$

where $L = \ell(\ell + 1)$ and ℓ is the usual angular momentum quantum number. E is the ro-vibrating energy states and $V_\pm(r)$ is the EP given by Eq. 1;

$$V_\pm(r) = D\{\delta - \varepsilon\,[coth(\eta r)]^{\pm 1}\}^2.$$

A more useful form of the EP is written in terms of hyperbolic functions

$$V_\pm(r) = D\left\{\delta^2 - 2\delta\varepsilon\left(\frac{1 \pm e^{-2\eta r}}{1 \mp e^{-2\eta r}}\right) + \varepsilon^2\left(\frac{1 \pm e^{-2\eta r}}{1 \mp e^{-2\eta r}}\right)^2\right\}. \tag{4}$$

If the L appeared in Eq. 3 is not too large, the following approximation can be used in place of the centrifugal term L/r^2 (or $\ell(\ell + 1)/r^2$) about the point of $r = r_e$

$$\frac{L}{r^2} \approx \frac{L}{r_e^2}\left\{A_0 + A_1\frac{\pm e^{-2\eta r}}{1 \mp e^{-2\eta r}} + A_2\left(\frac{\pm e^{-2\eta r}}{1 \mp e^{-2\eta r}}\right)^2\right\}, \tag{5}$$

where

$$A_0 = 1 - \left(\frac{1 \mp e^{-2\eta r_e}}{2\eta r_e}\right)^2 \left(\frac{8\eta r_e}{1 \mp e^{-2\eta r_e}} - 3 - 2\eta r_e\right), \tag{6}$$

$$A_1 = \pm 2\left(e^{2\eta r_e} \mp 1\right)\left\{3\left(\frac{1 \mp e^{-2\eta r_e}}{2\eta r_e}\right) - (3 + 2\eta r_e)\left(\frac{1 \mp e^{-2\eta r_e}}{2\eta r_e}\right)\right\}, \tag{7}$$

$$A_2 = \left(e^{2\eta r_e} \mp 1\right)^2 \left(\frac{1 \mp e^{-2\eta r_e}}{2\eta r_e}\right)^2 \left(3 + 2\eta r_e - \frac{4\eta r_e}{1 \mp e^{-2\eta r_e}}\right). \tag{8}$$

Substituting Eqs. 4 and 5 into Eq. 3, the radial equation becomes

$$\frac{d^2R(r)}{dr^2} - \frac{L}{r_e^2}\left\{A_0 + A_1\frac{\pm e^{-2\eta r}}{1 \mp e^{-2\eta r}} + A_2\left(\frac{\pm e^{-2\eta r}}{1 \mp e^{-2\eta r}}\right)^2\right\}R(r)$$
$$+\frac{2\mu}{\hbar^2}\left(E - D\left\{\delta^2 - 2\delta\varepsilon\left(\frac{1 \pm e^{-2\eta r}}{1 \mp e^{-2\eta r}}\right) + \varepsilon^2\left(\frac{1 \pm e^{-2\eta r}}{1 \mp e^{-2\eta r}}\right)^2\right\}\right)R(r) = 0. \tag{9}$$

Using a transformation $s = \pm e^{-2\eta r}$, Eq. 9 can be formed as an equation of hypergeometric type. This equation is written as

$$4\eta^2 s^2\frac{d^2R(s)}{ds^2} + 4\eta^2 s\frac{dR(s)}{ds} - \frac{L}{r_e^2}\left\{A_0 + A_1\frac{s}{1-s} + A_2\left(\frac{s}{1-s}\right)^2\right\}R(s)$$
$$+\frac{2\mu}{\hbar^2}\left(E - D\left\{\delta^2 - 2\delta\varepsilon\left(\frac{1+s}{1-s}\right) + \varepsilon^2\left(\frac{1+s}{1-s}\right)^2\right\}\right)R(s) = 0. \tag{10}$$

The further re-arrangements on Eq. 10 lead to the following equation

$$\frac{d^2R(s)}{ds^2} + \frac{1-s}{s(1-s)}\frac{dR(s)}{ds} + \frac{1}{s^2(1-s)^2}\left(Ks^2 + Qs + S\right)R(s) = 0, \tag{11}$$

where

$$K = \frac{\mu E}{2\eta^2\hbar^2} - \frac{L}{4\eta^2 r_e^2}(A_0 - A_1 + A_2) - \frac{\mu D}{2\eta^2\hbar^2}(\delta + \varepsilon)^2, \tag{12}$$

$$Q = -\frac{\mu E}{\eta^2\hbar^2} + \frac{L}{4\eta^2 r_e^2}(2A_0 - A_1) + \frac{\mu D}{\eta^2\hbar^2}(\delta^2 - \varepsilon^2), \tag{13}$$

$$S = \frac{\mu E}{2\eta^2\hbar^2} - \frac{LA_0}{4\eta^2 r_e^2} - \frac{\mu D}{2\eta^2\hbar^2}(\delta - \varepsilon)^2. \tag{14}$$

In order to solve Eq. 11 explicitly, the NU method can be used by following the basic equations given in Ref. [31]. To do this, Eq. 1 of Ref. [31] and Eq. 11 of the present study are compared with each other to determine the relevant polynomials;

$$\widetilde{\tau}(s) = 1 - s, \quad \sigma(s) = s(1-s), \quad \widetilde{\sigma}(s) = Ks^2 + Qs + S. \tag{15}$$

Inserting the polynomials given by Eq. 15 into Eq. 6 of Ref. [31], the polynomial $\pi(s)$ becomes

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2}\sqrt{s^2(1-4K-4k) + s(4k-4Q) - 4S}, \tag{16}$$

or

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2}\sqrt{\widetilde{a}x^2 + \widetilde{b}x + \widetilde{c}}, \tag{17}$$

where $\widetilde{a} = 1 - 4K - 4k, \widetilde{b} = 4k - 4Q$ and $\widetilde{c} = -4S$. According to the solution procedure of the NU method given in Ref. [31], the equation of quadratic form under the square root sign of Eq. 17 must be solved by setting the discriminant of this quadratic equal to zero: $\Delta = \widetilde{b}^2 - 4\widetilde{a}\widetilde{c} = 0$. The discriminant yields a new quadratic equation according to the constant k,

$$(k-Q)^2 + (1-4K-4k)S = 0, \tag{18}$$

or

$$k^2 - k(2Q+4S) + Q^2 + (1-4K)S = 0. \tag{19}$$

The solution of Eq. 19 gives us two roots

$$k_{\pm} = Q + 2S \pm \sqrt{S(4K+4Q+4S-1)}, \tag{20}$$

where the signs of plus and minus represent the roots of k_+ and k_-, respectively. When the individual values of k given in Eq. 20 are substituted into Eq. 16, the four possible forms of $\pi(s)$ are written as follows

$$\pi(s) = -\frac{s}{2} \pm \frac{i}{2}\begin{cases} \left[\left(2\sqrt{S} + \sqrt{4K+4Q+4S-1}\right)s - 2\sqrt{S}\right], \\ \text{for} \quad k_+ = Q + 2S + \sqrt{S(4K+4Q+4S-1)} \\ \left[\left(2\sqrt{S} - \sqrt{4K+4Q+4S-1}\right)s - 2\sqrt{S}\right]. \\ \text{for} \quad k_- = Q + 2S - \sqrt{S(4K+4Q+4S-1)} \end{cases} \tag{21}$$

One of the four values of the polynomial $\pi(s)$ is just proper to obtain the ro-vibrating energy states because $\tau(s)$ given by Eq. 9 of Ref. [31] has a negative derivative for this value of $\pi(s)$. Therefore, the most suitable form of $\pi(s)$ is chosen as

$$\pi(s) = -\frac{s}{2} - \frac{i}{2}\left[\left(2\sqrt{S} - \sqrt{4K+4Q+4S-1}\right)s - 2\sqrt{S}\right] \tag{22}$$

for $k_- = Q + 2S - \sqrt{S(4K + 4Q + 4S - 1)}$. Hence, $\tau(s)$ and $\tau'(s)$ are obtained, respectively,

$$\begin{aligned}\tau(s) &= 1 + 2i\sqrt{S} - s\left(2 + 2\sqrt{\frac{LA_2}{4\eta^2 r_e^2} + \frac{2\mu D}{\eta^2\hbar^2}\varepsilon^2 + \frac{1}{4}} + 2i\sqrt{S}\right),\\ \tau'(s) &= -\left(2 + 2\sqrt{\frac{LA_2}{4\eta^2 r_e^2} + \frac{2\mu D}{\eta^2\hbar^2}\varepsilon^2 + \frac{1}{4}} + 2i\sqrt{S}\right) < 0\,.\end{aligned} \tag{23}$$

where $\tau'(s)$ represents the derivative of $\tau(s)$. To obtain a particular solution through the NU method, the expressions of λ and λ_n are calculated by using the equalities of $\lambda = k_- + \pi'(s)$ and $\lambda_n = -n\tau'(s) - (n(n-1)/2)\sigma''(s)$, where n is the number of nodes of the radial wave function $R(r)$. Consequently, these equalities are determined

$$\begin{aligned}\lambda = {} & \frac{2\mu D}{\eta^2\hbar^2}\varepsilon(\delta - \varepsilon) - \frac{LA_1}{4\eta^2 r_e^2} - 2i\sqrt{S}\sqrt{\frac{LA_2}{4\eta^2 r_e^2} + \frac{2\mu D}{\eta^2\hbar^2}\varepsilon^2 + \frac{1}{4}}\\ & -\frac{1}{2} - i\sqrt{S} - \sqrt{\frac{LA_2}{4\eta^2 r_e^2} + \frac{2\mu D}{\eta^2\hbar^2}\varepsilon^2 + \frac{1}{4}},\end{aligned} \tag{24}$$

$$\lambda_n = n + n^2 + 2n\sqrt{\frac{LA_2}{4\eta^2 r_e^2} + \frac{2\mu D}{\eta^2\hbar^2}\varepsilon^2 + \frac{1}{4}} + 2ni\sqrt{S}. \quad (n = 0, 1, 2, \ldots) \tag{25}$$

With $\lambda = \lambda_n$, the ro-vibrating energy states are obtained for a diatomic molecule

$$\begin{aligned}E \equiv E^{n\ell}_{\pm} = {} & D(\delta - \varepsilon)^2 + \frac{\hbar^2 LA_0}{2\mu r_e^2} - \frac{\eta^2\hbar^2}{2\mu}\\ & \left[\frac{\frac{2\mu D}{\eta^2\hbar^2}\varepsilon(\delta - \varepsilon) - \frac{LA_1}{4\eta^2 r_e^2} - \frac{1}{4} - 2\left(n + \frac{1}{2}\right)\sqrt{\frac{LA_2}{4\eta^2 r_e^2} + \frac{2\mu D}{\eta^2\hbar^2}\varepsilon^2 + \frac{1}{4}} - \left(n + \frac{1}{2}\right)^2}{n + \frac{1}{2} + \sqrt{\frac{LA_2}{4\eta^2 r_e^2} + \frac{2\mu D}{\eta^2\hbar^2}\varepsilon^2 + \frac{1}{4}}}\right]^2,\end{aligned} \tag{26}$$

keeping in mind $L = \ell(\ell + 1)$. The result obtained in Eq. 26 is also agrement with that of Ref. [39]. The upper indices n and ℓ of $E^{n\ell}_{\pm}$ represent the quantum numbers whereas the lower ones ± comes from the two different forms of the EP. The physically valid values of the ro-vibrating energy states are given by low values of δ and ε for $V_-(r)$ or high values of δ and ε for $V_+(r)$ [32]. Of course, it is clear that by imposing appropriate changes in the parameters of EP and keeping the constants D_e and r_e for some molecules, the ro-vibrating energy states can be calculated by using Eq. 26.

3 Numerical applications

In order to test the accuracy of Eq. 26, the ro-vibrating energy states of the molecules $^1H_2$ and $^{40}Ar_2$ are calculated as a numerical example. The spectroscopic constants

Table 1 The spectroscopic constants of the EP listed in this table are taken from Ref. [32]

Parameters	H_2	Ar_2
$D_e(\mathrm{cm}^{-1})$	38281	99.55
$r_e(\text{Å})$	0.7414	3.7590
μ(a.u)	0.50407	19.9812

Table 2 The potential parameters of H_2 molecule in the EP ($V_\pm(r)$)

	EP	ε	δ	η (Å^{-1})	$E_\pm(SC)$	$E_\pm(QM)$	$E_\pm(NU)$
(1)	$V_-(r)$	−19.228	−0.961	1.8520	2171.70	2142.84	2142.84
(2)		−31.702	−9.235	1.5059	2176.71	2159.74	2159.74
(3)		−86.175	−57.223	1.1686	2173.96	2167.73	2167.73
(4)		−410.090	−376.710	1.0135	2170.23	2168.93	2168.93
(5)	$V_+(r)$	426.826	463.102	0.9327	2167.68	2168.93	2168.93
(6)		47.294	102.341	0.6146	2153.69	2164.83	2164.83
(7)		28.685	117.121	0.3826	2139.57	2157.69	2157.69
(8)		21.250	213.212	0.1762	2124.29	2148.40	2148.40

Semiclassically (SC) and quantum mechanically (QM) calculated energy eigenvalues (cm^{-1}) for the ground state $n = 0$ ($E_\pm(SC)$ and $E_\pm(QM)$) are taken from Ref. [32] and their results are compared with those of the NU method ($E_\pm(NU)$)

which is used in the numerical calculations of the selected molecules are given in Table 1. The first calculation is applied to the molecule H_2. The ro-vibrating energy states of the H_2 in the EP (for both $V_+(r)$ and $V_-(r)$) for $n = 0$ and $\ell = 0$ are determined with the NU method by using the relevant potential parameters given in Table 2. The numerical results obtained by the NU method are listed in Table 2 and compared with the results obtained by a semiclassical (SC) procedure (the Bohr-Sommerfeld quantization condition) and a quantum mechanical (QM) method pointed in Ref. [32]. In Table 2, $E_\pm(SC)$ and $E_\pm(QM)$ represent the semiclassical and quantum mechanical energy eigenvalues, respectively, for the ground state $n = 0$. $E_\pm(NU)$ indicates the results obtained by using the NU method for the same ground state. It is seen that from Table 2 the results obtained by means of the NU method are also agrement with those obtained by a quantum mechanical method whereas the semiclassical procedure is proportionally different. To attain the best representation of the ro-vibrating energy states, the values of the potential parameters of $V_\pm(r)$ are changed systematically from high values to low ones. These variations are the best appropriate for $V_-(r)$ with low values of δ and ε or for $V_+(r)$ with high values of δ and ε. Therefore, the differences between the ro-vibrating energy states calculated by the NU method and semiclassical procedure are less than 0.01 cm^{-1}, i.e. they are negligible small.

The second calculation is applied to the molecule Ar_2. The obtained results are only discussed for the ro-vibrating energy states in $V_+(r)$ because the potential parameters of $V_+(r)$ were fitted with the spectroscopic constants given in Table 1. The parameters and their values which are used in numerical calculations are $\varepsilon = 25.23$, $\delta = 41.75$ and $\eta = 0.6604$ Å^{-1} [32]. The ro-vibrating energy states obtained by the NU method

Table 3 Comparisons of experimentally determined values with the results of the SC procedure and the NU method for the transition $n \neq 0 \rightarrow n = 0$ in the case of $\ell = 0$

n	$\triangle E1$	$\triangle E2$	$\triangle E3$	$\triangle E4$	$\triangle E_+(SC)$	$\triangle E_+(NU)$
1	25.74	25.49	25.21	25.56	25.75	25.72
2	46.15	45.63	45.02	46.00	46.01	45.95
3	61.75	60.70	60.04	61.32	61.42	61.33
4	72.66	71.33	70.92	71.52	72.52	72.42
5	79.44	–	–	–	79.79	79.66
6	–	–	–	–	83.59	83.45

The differences between the energy states are in cm^{-1}

and semiclassical procedure are presented in Table 3 with the differences $\triangle E_+ = E_+(n \neq 0) - E_+(n = 0)$ and compared with experimentally determined values which are taken from the relevant references of Ref. [32]. In Table 3, the $\triangle E1$, $\triangle E2$, $\triangle E3$ and $\triangle E4$ represent four-different experimental results whereas $\triangle E_+(SC)$ and $\triangle E_+(NU)$

Table 4 The ro-vibrating energy states (in cm^{-1}) corresponding to the several values of n and ℓ for H_2 and Ar_2 molecules in $V_+(r)$

n	ℓ	$E_+(for\ H_2)$	$E_+\ (for\ Ar_2)$
0	0	2168.93	15.3185
1	0	6307.41	41.0395
	1	6308.22	23.7236
2	0	10185.1	61.2667
	1	10187.0	47.8706
	2	10190.9	2.8187
3	0	13803.7	76.6516
	1	13806.9	66.6379
	2	13813.1	31.7756
	3	13822.3	–
4	0	17165.3	87.7380
	1	17169.6	80.6749
	2	17178.1	54.5210
	3	17190.8	–
	4	17207.6	–
5	0	20271.7	94.9827
	1	20277.1	90.5216
	2	20287.8	71.8969
	3	20303.9	–
	4	20325.2	–
	5	20351.8	–

The results are obtained by using the Nikiforov–Uvarov method show the results of the semiclassical procedure and the NU method, respectively. It is seen that from Table 3 the results obtained by the NU method are also agrement with experimentally determined values as well as the semiclassical procedure.

The further calculations on the H_2 and Ar_2 molecules are also given for the non-zero values of ℓ, i.e. $\ell \neq 0$. In Table 4, we present the ro-vibrating energy states in the potential $V_{+}(r)$ for relatively low values of vibrational ($n = 0, 1, 2, 3, 4, 5$) and rotational ($\ell = 0, 1, 2, 3, 4, 5$) quantum numbers. The first calculation in the table dedicates to the molecule H_2 in the potential $V_{+}(r)$. The results obtained for the H_2 clearly indicate that the approximation used in this study to determine the ro-vibrating energy states gives the results of reasonable accuracy for those fairly small quantum numbers, considering the first six values of n and ℓ. The second calculation of the table relates to the molecule Ar_2 in the same potential. Although the approximation loess its accuracy for the high ro-vibrational states, it is consistently much better for the states of $\ell = 0, 1, 2$.

4 Conclusions

We have presented an useful approximation to obtain the ro-vibrating energy states of a diatomic molecule in an empirical potential. To solve the Schrödinger equation approximately, the Nikiforov–Uvarov (NU) method is used by reducing this equation to the differential equation of the hypergeometric type, after having make an appropriate coordinate transformation. The method taken into account in this study is systematical and efficient in finding the eigenvalues of the Schrödinger equation for various diatomic molecules. The main result obtained by means of the NU method is summarized in Eq. 26, considering the approximation given by Eq. 5. The validity of the result is tested by calculating the ro-vibrating energy states of the molecules H_2 and Ar_2. Comparisons with the results of previous methods (SC and QM) for the ground state $n = 0$ and $\ell = 0$ indicate that the energy expression given by Eq. 26 is consistently agrement with those obtained by these methods, without considering the small differences come from the SC procedure. It is seen that the energy expression is compatible with experimental results for fairly high values of the ro-vibrating energy states of the molecule H_2 whereas in the case of Ar_2 it is only permissible for low values of the ro-vibrating energy states, i.e. $\ell = 0, 1, 2$. Finally, the presented approximation could be useful for other molecular potentials in calculating their higher or lower ro-vibrating energy states.

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