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Thermodynamic properties and the approximate solutions of the Schrödinger equation with the shifted Deng–Fan potential model

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With the introduction of a new improved approximation scheme (Pekeris-type approximation) to deal with the centrifugal term, the energy eigenvalues and the wave functions of the Schrödinger equation of the shifted Deng–Fan molecular potential are obtained, via the asymptotic iteration method. Rotational–vibrational energy eigenvalues of some diatomic molecules are presented, these results are in good agreement with other results in the literature. For these selected diatomic molecules, energy eigenvalues obtained are in much better agreement with the results obtained from the rotating Morse potential model for moderate values of rotational and vibrational quantum numbers. Furthermore, thermodynamic properties such as the vibrational mean U , specific heat C , free energy F and entropy S for the pure vibrational state in the classical limit for these energy eigenvalues are studied.

Keywords: shifted Deng–Fan molecular potential; Pekeris-type approximation; asymptotic iteration; eigenvalues; eigenfunction; partition function

1. Introduction

The molecular Deng–Fan potential is a simple modified Morse potential, also known as the generalised Morse potential that was proposed by Deng and Fan half a century ago [1]. This was done in an attempt to find a more suitable diatomic potential to describe the vibrational spectrum [2], qualitatively similar to the Morse potential with the correct asymptotic behaviour as the inter-nuclear distance approaches zero. This potential model can be used to describe the motion of the nucleons in the mean field produced by the interactions between nuclei [3]. This potential has been used to describe diatomic molecular energy spectra and electromagnetic transitions and it is an ideal inter-nuclear potential in diatomic molecules with the same behaviour for $r \rightarrow 0$ [1–9]. Because of its importance in chemical physics, molecular spectroscopy, molecular physics and related areas, the bound state solutions of the relativistic and non-relativistic wave equations have been studied by several authors [4–12].

The approximate solutions of the relativistic (Klein–Gordon and Dirac) equations with the Deng–Fan potential, including the centrifugal term via the Nikiforov–Uvarov method have been obtained by Oluwadare et al. [9], a solution of the spinless particle (for $\ell = 0$) has also been obtained [4]. Zhang et al. [8] used a new improved approximation scheme to deal with the centrifugal term of the

Schrödinger equation of the generalised Morse potential model (that is, Deng–Fan potential) to obtain the approximate solutions via the SUSY approach, the results obtained are in better agreement with the other results obtained by using other methods [8].

Also, some investigations have been carried out for other related molecular potential models. For instance, the improved expressions for the Schiöberg potential energy models for diatomic molecules have been obtained by Wang et al. (2012a). They found that none of the six three-parameter empirical potential energy functions (both versions of the Schiöberg potential functions; Rosen–Morse and Manning–Rosen functions) is superior to the other potentials in fitting experimental data for the molecules examined [12].

In addition, the equivalence of the Wei potential model and Tietz potential model for diatomic molecules has been investigated by Jia et al. [13]. It was found that the Tietz potential function is a four-parameter potential function, and that the Wei potential energy function and Tietz potential energy function are the same solvable empirical potential energy function for diatomic molecules [13].

Furthermore, Wang et al. (2012b) found that the three empirical potential energy models (Deng–Fan potential inclusive) for diatomic molecules are equivalent, their results show that the Manning–Rosen, Deng–Fan and Schiöberg

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potentials are not better than the traditional Morse potential in stimulating the atomic interaction for diatomic molecules [14].

In order to overcome this observation of Wang et al., Hamzavi et al. (2012) suggested a modification to the Deng–Fan potential, called the shifted Deng–Fan potential [10]. The shifted Deng–Fan potential examined in this study is the Deng–Fan potential shifted by dissociation energy D_2 [10]. Hamzavi et al. (2012) studied the Schrödinger equation with this potential and applied their results to some diatomic molecules [10]. From their plot for the shifted Deng–Fan potential and the Morse potential using the parameters set for H_2 diatomic molecule, it is obvious that the two potentials are very close to each other for large values of r in the regions $r \approx r_e$ and $r > r_e$, but they are very different at $r \approx 0$. Also, if both the Deng–Fan and the shifted Deng–Fan potentials are deep (that is, $D \gg 1$) they could be well approximated by a harmonic oscillator in the region $r \approx r_e$ [10].

Recently, thermodynamic properties of liquid alkali metals have been investigated via the pseudopotential perturbation scheme. In this study, a new model potential has been used with the exchange and correlation effect to calculate internal energy (enthalpy), entropy and Helmholtz free energy of liquid Na, K, Rb and Cs at various temperatures with the variational approach [15]. In a similar manner, Dong et al. (2007) studied the hidden symmetries and thermodynamic properties for a harmonic oscillator plus an inverse square potential [16]. Also, the energy spectrum and the thermodynamic properties for a modified Rosen–Morse potential have been obtained by using the proper quantisation rule by Dong and Cruz–Irisson [17].

The purpose of the present work is threefolds. First, we introduce an alternative method called the asymptotic iteration method (AIM) for an algebraic solution of the Schrödinger equation with this potential [18–27]. Using this method and by introducing the Pekeris-type approximation scheme to deal with the centrifugal term, we obtain analytical approximation to the ℓ -wave solutions of the Schrödinger equation. Second, we compute eigenvalues numerically for rotational and vibrational quantum numbers n and ℓ with applications to some diatomic molecules. A special case of the potential is also examined (that is, the Deng–Fan potential). A comparison of our numerical results with other methods reveals that AIM is accurate, efficient and reliable. Finally, a vibrational high temperature partition function is presented. Some thermodynamic functions are derived and their properties are studied.

2. Method of analysis

One of the calculation tools utilised in solving the Schrödinger-like equation, including the centrifugal barrier and/or the spin-orbit coupling (or pseudospin-orbit coupling) term is the asymptotic iteration method (AIM)

[18–29]. For a given potential the idea is to convert the Schrödinger-like equation to the homogeneous linear second-order differential equation of the form:

$$y''(x) = \lambda_o(x)y'(x) + s_o(x)y(x), \quad (1)$$

where $\lambda_o(x)$ and $s_o(x)$ have sufficiently many continuous derivatives and defined in some interval that are not necessarily bounded. Differential Equation (1) has a general solution [24]

$$y(x) = \exp\left(-\int^x \alpha(x')dx'\right) \left[C_2 + C_1 \times \int^x \exp\left(\int^{x'} [\lambda_o(x'') + 2\alpha(x'')]dx''\right)dx' \right]. \quad (2)$$

If $k > 0$, for sufficiently large k , we obtain the $\alpha(x)$

$$\frac{s_k(x)}{\lambda_k(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} = \alpha(x), \quad k = 1, 2, 3, \dots \quad (3)$$

where

$$\lambda_k(x) = \lambda'_{k-1}(x) + s_{k-1}(x) + \lambda_o(x)\lambda_{k-1}(x)$$

$$s_k = s'_{k-1}(x) + s_o(x)\lambda_{k-1}(x), \quad k = 1, 2, 3, \dots \quad (4)$$

With the quantisation condition

$$\delta_k(x) = \begin{vmatrix} \lambda_k(x) & s_k(x) \\ \lambda_{k-1}(x) & s_{k-1}(x) \end{vmatrix} = 0, \quad k = 1, 2, 3, \dots \quad (5)$$

The energy eigenvalues are then obtained from Equation (5), if the problem is exactly solvable.

3. Applications

3.1. Bound-state solutions of the Schrödinger equation with the shifted Deng–Fan potential

The shifted Deng–Fan exponential-type potential that is under investigation in this investigation is defined as [10]

$$V(r) = D_1 \left(1 - \frac{b}{e^{ar} - 1}\right)^2 - D_2, \quad b = e^{ar_e} - 1, \quad (6)$$

where (D_1, D_2) , b and a are three parameters representing the dissociation energy, the position of the minimum r_e and the radius of the potential, respectively. This potential is a form of the Deng–Fan potential [1–9]. A variation of the shifted Deng–Fan potential with the Deng–Fan and Morse potentials for H_2 diatomic molecule is as shown in Figure 1.

Inserting this potential into the Schrödinger equation, the radial part of the Schrödinger equation takes the

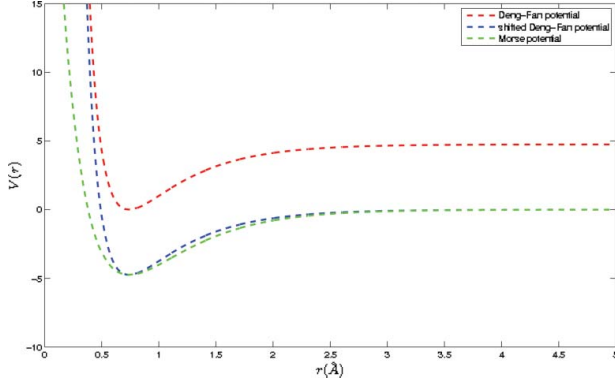


Figure 1. The behaviour of the shifted Deng–Fan potential with respect to the Deng–Fan and Morse potentials for H_2 diatomic molecule.

following form:

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \left[\frac{2m(E_{n\ell} + D_2)}{\hbar^2} - \frac{2mD_1}{\hbar^2} \left(1 - \frac{b}{e^{ar} - 1} \right)^2 - \frac{\ell(\ell + 1)}{r^2} \right] R_{n\ell}(r). \quad (7)$$

Radial wave Equation (7) is an exactly solvable problem for s -wave [4]. For ℓ -wave states, the problem is not analytically solvable and therefore we have to use an approximation to deal with the centrifugal term [3–9, 18–20, 26, 30]. It is noted that for a short potential range, the following formula is a proper approximation to $1/r^2$:

$$\frac{1}{r^2} \approx a^2 \left[C_o + \frac{e^{ar}}{(e^{ar} - 1)^2} \right], \quad (8)$$

where $C_o = \frac{1}{12.0015}$. It is pertinent to note that when $C_o = 0$, this approximation scheme reduces to the one used by Dong and Gu [6], Dong et al. (2007) [31] and Qiang and Dong (2007) [32]. With the help of Equation (8) and by introducing the change in variable $r \rightarrow \varrho$ through mapping function $\varrho = (e^{ar} - 1)^{-1}$, Equation (7) thus becomes

$$\begin{aligned} & \varrho^2(1 + \varrho)^2 \frac{d^2 R_{n\ell}(\varrho)}{d\varrho^2} + \varrho(1 + 2\varrho)(1 + \varrho) \frac{dR_{n\ell}(\varrho)}{d\varrho} \\ &= - \left\{ \varrho^2 \left(\ell(\ell + 1) - \frac{2mb^2 D_1}{\hbar^2 a^2} \right) + \varrho \left(\frac{4bmD_1}{\hbar^2 a^2} \right) \right. \\ & \quad \left. + \left(\frac{2m}{\hbar^2 a^2} (E_{n\ell} + D_2) - C_o \ell(\ell + 1) \right) \right\} R_{n\ell}(\varrho). \quad (9) \end{aligned}$$

It is well known that the singularity points of the above Equation (9) plays an important role in the form of the wave functions. The singularity points here are at $\varrho = 0$ and at $\varrho = -1$. As a result, we take wave function of

the form

$$R_{n\ell}(\varrho) = \varrho^\gamma (1 + \varrho)^{-\epsilon} f_{n\ell}(\varrho), \quad (10)$$

where

$$\begin{aligned} \gamma &= \left[\frac{2mD_1}{\hbar^2 a^2} + \frac{\ell(\ell + 1)}{12.0015} - \frac{2m}{\hbar^2 a^2} (E_{n\ell} + D_2) \right]^{\frac{1}{2}}, \\ \epsilon &= \left[\frac{2mD_1}{\hbar^2 a^2} (b^2 + 1) + \frac{4mbD_1}{\hbar^2 a^2} + C_o \ell(\ell + 1) \right]^{\frac{1}{2}}. \quad (11) \end{aligned}$$

Substitution of Equation (10) into Equation (9) leads to the following equations

$$\begin{aligned} & \frac{d^2 f_{n\ell}(\varrho)}{d\varrho^2} + \left[\frac{2(\gamma - \epsilon + 1) + (1 + 2\gamma)}{\varrho(1 + \varrho)} \right] \frac{df_{n\ell}(\varrho)}{d\varrho} \\ &+ \left[\frac{(\gamma - \epsilon)^2 + (\gamma - \epsilon) - \frac{2mb^2 D_1}{\hbar^2 a^2} - \ell(\ell + 1)}{\varrho(1 + \varrho)} \right] f_{n\ell}(\varrho), \quad (12) \end{aligned}$$

which is now in a suitable form to apply the asymptotic iteration method. By comparing this equation with Equation (1), we can write $\lambda_0(\varrho)$ and $s_0(\varrho)$ as

$$\begin{aligned} \lambda_0(\varrho) &= - \left[\frac{2(\gamma - \epsilon + 1) + (1 + 2\gamma)}{\varrho(1 + \varrho)} \right], \\ s_0(\varrho) &= - \left[\frac{(\gamma - \epsilon)^2 + (\gamma - \epsilon) - \frac{2mb^2 D_1}{\hbar^2 a^2} - \ell(\ell + 1)}{\varrho(1 + \varrho)} \right]. \quad (13) \end{aligned}$$

With the help of Equation (4) and the quantisation condition given in Equation (5), we arrive at the following eigenvalue relations

$$\begin{aligned} \delta_0(\varrho) &= \begin{vmatrix} \lambda_1(\varrho) & s_1(\varrho) \\ \lambda_0(\varrho) & s_0(\varrho) \end{vmatrix} = 0 \\ \Rightarrow \epsilon_0 - \gamma_0 &= \frac{1}{2} + \frac{1}{2} \sqrt{1 + 4 \left(\frac{2mb^2 D_1}{\hbar^2 a^2} + \ell(\ell + 1) \right)}, \\ \delta_1(\varrho) &= \begin{vmatrix} \lambda_2(\varrho) & s_2(\varrho) \\ \lambda_1(\varrho) & s_1(\varrho) \end{vmatrix} = 0 \\ \Rightarrow \epsilon_1 - \gamma_1 &= \frac{3}{2} + \frac{1}{2} \sqrt{1 + 4 \left(\frac{2mb^2 D_1}{\hbar^2 a^2} + \ell(\ell + 1) \right)}, \\ \delta_2(\varrho) &= \begin{vmatrix} \lambda_3(\varrho) & s_3(\varrho) \\ \lambda_2(\varrho) & s_2(\varrho) \end{vmatrix} = 0 \\ \Rightarrow \epsilon_2 - \gamma_2 &= \frac{5}{2} + \frac{1}{2} \sqrt{1 + 4 \left(\frac{2mb^2 D_1}{\hbar^2 a^2} + \ell(\ell + 1) \right)}. \quad (14) \end{aligned}$$

Generalising the above expression and using the abbreviations in Equation (11), the eigenvalues become

$$E_{n\ell} = \frac{a^2 \hbar^2}{2m} \left\{ \left[\frac{2mD_1}{a^2 \hbar^2} (b+1)^2 + C_o \ell(\ell+1) \right] - \left[\frac{\frac{2mD_1}{a^2 \hbar^2} [(b+1)^2 - 1] + \left(\sqrt{\left(\ell + \frac{1}{2}\right)^2 + \frac{2mb^2 D_1}{a^2 \hbar^2} + \frac{2n+1}{2}} \right)^2}{2\sqrt{\left(\ell + \frac{1}{2}\right)^2 + \frac{2mb^2 D_1}{a^2 \hbar^2} + \frac{2n+1}{2}}} \right]^2 \right\} - D_2. \quad (15)$$

Also, we can obtain the eigenvalue expressions for a special case where $D_2 = 0$ (Deng–Fan).

For a calculation of the wave functions, the differential equation to be solved is transformed into the form [24,25]:

$$y''(x) = 2 \left(\frac{tx^{N+1}}{1-bx^{N+2}} - \frac{p+1}{x} \right) y'(x) - \frac{Wx^N}{1-bx^{N+2}}, \quad (16)$$

where t , b and p are arbitrary constants. A general solution of Equation (16) is found as [24,25]

$$y_n(x) = (-1)^n C_2(N+2)^n (\sigma)_n {}_2F_1(-n, \rho + n; \sigma; bx^{N+2}), \quad (17)$$

where the following notations have been used

$$\begin{aligned} (\sigma)_n &= \frac{\Gamma(\sigma + n)}{\Gamma(\sigma)}, \quad \sigma = \frac{2p + N + 3}{N + 2} \text{ and} \\ \rho &= \frac{(2p + 1)b + 2t}{(N + 2)b}. \end{aligned} \quad (18)$$

Now, comparing Equations (16) and (12), we have $t = \beta - \frac{1}{2}$, $b = -1$, $N = -1$, $p = \gamma - \frac{1}{2}$, $\sigma = 2\gamma + 1$, $\rho = 2(\gamma - \epsilon) + 1$ and then the solution of Equation (12) can easily be obtained as

$$\begin{aligned} f_{n\ell}(\varrho) &= (-1)^n C_2 \frac{\Gamma(2\gamma + n + 1)}{\Gamma(2\gamma + 1)} {}_2F_1(-n, 2(\gamma - \epsilon) + n + 1; \\ &2\gamma + 1; -\varrho), \end{aligned} \quad (19)$$

where Γ and ${}_2F_1$ are the Gamma function and hypergeometric function, respectively. By using Equations (19) and (10), the total radial wave function can be written as follows:

$$\begin{aligned} R_{n\ell}(r) &= N_{n\ell} \left(\frac{(e^{ar} - 1)^\gamma}{(1 - e^{-ar})^\epsilon} \right) {}_2F_1(-n, 2(\gamma - \beta) + n + 1; \\ &2\gamma + 1; -(e^{ar} - 1)^{-1}), \end{aligned} \quad (20)$$

where $N_{n\ell}$ is the normalisation constant.

3.2. Thermodynamic properties of the Schrödinger equation with the shifted Deng–Fan potential

In order to study the thermodynamic properties of this model potential in which the pure vibrational states have

been considered, we derive the eigenvalue E_n as:

$$\begin{aligned} E_n &= \frac{a^2 \hbar^2}{2m} \left[A - \left(\frac{B}{2(n+c)} + \frac{n+c}{2} \right)^2 \right], \\ n &= 0, 1, 2, \dots, < [-c + \sqrt{A} \pm \sqrt{A-B}], \end{aligned} \quad (21)$$

$[-c + \sqrt{A} \pm \sqrt{A-B}]$ means the largest integer inferior to $-c + \sqrt{A} \pm \sqrt{A-B}$. We have introduced the following notations for simplicity:

$$\begin{aligned} A &= \frac{2m}{a^2 \hbar^2} [D_1(b+1)^2 - D_2], \quad B = \frac{2mD_1}{a^2 \hbar^2} [(b+1)^2 - 1], \\ c &= \frac{1}{2} \left[1 + \sqrt{1 + 4 \left(\frac{2mb^2 D_1}{a^2 \hbar^2} \right)} \right], \end{aligned} \quad (22)$$

and the vibrational partition function is obtained as

$$\begin{aligned} Z_{vib}(\beta) &= \sum_{n=0}^{\lambda} e^{-\beta E_n}, \quad \beta = \frac{1}{kT}, \\ \lambda &= -c + \sqrt{A} \pm \sqrt{A-B}, \end{aligned} \quad (23)$$

where k is the Boltzmann constant. By substituting Equation (21) into Equation (23), the partition function for this potential is obtained as

$$Z_{vib}(\beta) = \sum_{n=0}^{\lambda} e^{\frac{\beta a^2 \hbar^2}{4m} (B-2A) + \frac{\beta a^2 \hbar^2 B^2}{8m(n+c)^2} + \frac{\beta a^2 \hbar^2}{8m} (n+c)^2}. \quad (24)$$

In the classical limit, the sum can be replaced by an integral, such that

$$\begin{aligned} Z_{vib}(\beta) &= \int_0^{\lambda} e^{\frac{\beta a^2 \hbar^2}{4m} (B-2A) + \frac{\beta a^2 \hbar^2 B^2}{8m(n+c)^2} + \frac{\beta a^2 \hbar^2}{8m} (n+c)^2} dn, \\ &= \int_c^{\lambda+c} e^{\frac{\beta a^2 \hbar^2}{4m} (B-2A) + \frac{\beta a^2 \hbar^2 B^2}{8m\rho^2} + \frac{\beta a^2 \hbar^2}{8m} \rho^2} d\rho, \quad \rho = c + n, \\ &= e^{\beta \Lambda_3} \sqrt{\pi} \left[\frac{[1 - \text{Erf}(\Lambda_1 \sqrt{\beta})] - e^{\Lambda_4 \beta} [1 - \text{Erf}(\Lambda_2 \sqrt{\beta})]}{\Lambda_5 \sqrt{\beta}} \right], \end{aligned} \quad (25)$$

where we have also introduced the following parameters for mathematical simplicity,

$$\begin{aligned}\Lambda_1 &= \frac{1}{\rho} \sqrt{-\frac{a^2 \hbar^2 B^2}{8m}} - \rho \sqrt{-\frac{a^2 \hbar^2}{8m}}, \quad \Lambda_2 = \frac{1}{\rho} \sqrt{-\frac{a^2 \hbar^2 B^2}{8m}} + \rho \sqrt{-\frac{a^2 \hbar^2}{8m}} \\ \Lambda_3 &= -\frac{a^2 \hbar^2 A}{2m}, \quad \Lambda_4 = \frac{a^2 \hbar^2 B}{2m}, \quad \Lambda_5 = \sqrt{-2a^2 \hbar^2}, \quad c \leq \rho \leq c + \lambda.\end{aligned}\quad (26)$$

Having determined the vibrational partition function, we can easily obtain the thermodynamic properties for the model potential as follows:

(1) The vibrational mean energy U :

$$\begin{aligned}U(\beta) &= -\frac{\partial}{\partial \beta} \ln Z_{vib}(\beta) \\ &= e^{-\beta \Lambda_1^2} \left\{ -\frac{2\sqrt{\beta} (\Lambda_1 - \Lambda_2 e^{\beta(\Lambda_1^2 - \Lambda_2^2 + \Lambda_4)})}{2\beta \sqrt{\pi} [\text{Erfc}(\Lambda_1 \sqrt{\beta}) - e^{\beta \Lambda_4} \text{Erfc}(\Lambda_2 \sqrt{\beta})]} \right. \\ &\quad \left. - \frac{e^{\beta \Lambda_1^2} \sqrt{\pi} ((1 - 2\beta \Lambda_3) \text{Erfc}(\sqrt{\beta} \Lambda_1) + e^{\beta \Lambda_4} (-1 + 2\beta(\Lambda_3 + \Lambda_4)) \text{Erfc}(\sqrt{\beta} \Lambda_2))}{2\beta \sqrt{\pi} [\text{Erfc}(\Lambda_1 \sqrt{\beta}) - e^{\beta \Lambda_4} \text{Erfc}(\Lambda_2 \sqrt{\beta})]} \right\}.\end{aligned}\quad (27)$$

(2) Vibrational specific heat C :

$$\begin{aligned}C(\beta) &= \frac{\partial}{\partial T} U = -k\beta^2 \frac{\partial}{\partial \beta} U = k e^{-\beta(2\Lambda_1^2 + \Lambda_3^2)} \left\{ \frac{e^{-\beta(2\Lambda_1^2 + \Lambda_3^2)}}{2\pi [\text{Erfc}(\sqrt{\beta} \Lambda_1) - e^{\beta \Lambda_4} \text{Erfc}(\sqrt{\beta} \Lambda_2)]^2} \right. \\ &\quad + \frac{\sqrt{\pi} \text{Erfc}(\sqrt{\beta} \Lambda_1) \left[\sqrt{\beta} e^{\beta \Lambda_1^2} (e^{\beta \Lambda_2^2} (\Lambda_1 + 2\beta \Lambda_1^3) - e^{\beta(\Lambda_1^2 + \Lambda_4)} \Lambda_2 (1 + 2\beta \Lambda_2^2 - 4\beta \Lambda_4)) \right]}{2\pi [\text{Erfc}(\sqrt{\beta} \Lambda_1) - e^{\beta \Lambda_4} \text{Erfc}(\sqrt{\beta} \Lambda_2)]^2} \\ &\quad + \frac{\left[\sqrt{\pi} \text{Erfc}(\sqrt{\beta} \Lambda_2) \sqrt{\beta} e^{\beta(\Lambda_1^2 + \Lambda_4)} (e^{\beta(\Lambda_1^2 + \Lambda_4)} (\Lambda_2 + 2\beta \Lambda_2^3) - e^{\beta \Lambda_2^2} \Lambda_1 (1 + 2\beta \Lambda_1^2 + 4\beta \Lambda_4)) \right]}{2\pi [\text{Erfc}(\sqrt{\beta} \Lambda_1) - e^{\beta \Lambda_4} \text{Erfc}(\sqrt{\beta} \Lambda_2)]^2} \\ &\quad - \frac{(\sqrt{\pi} \text{Erfc}(\sqrt{\beta} \Lambda_1) 2e^{\beta(2\Lambda_1^2 + \Lambda_2^2 + \Lambda_4)} (1 + \beta^2 \Lambda_4^2) \sqrt{\pi} \text{Erfc}(\sqrt{\beta} \Lambda_2))}{2\pi [\text{Erfc}(\sqrt{\beta} \Lambda_1) - e^{\beta \Lambda_4} \text{Erfc}(\sqrt{\beta} \Lambda_2)]^2} \\ &\quad \left. - \frac{(\sqrt{\pi} \text{Erfc}(\sqrt{\beta} \Lambda_1) 2e^{\beta(2\Lambda_1^2 + \Lambda_2^2 + \Lambda_4)} (1 + \beta^2 \Lambda_4^2) \sqrt{\pi} \text{Erfc}(\sqrt{\beta} \Lambda_2))}{2\pi [\text{Erfc}(\sqrt{\beta} \Lambda_1) - e^{\beta \Lambda_4} \text{Erfc}(\sqrt{\beta} \Lambda_2)]^2} \right\}.\end{aligned}\quad (28)$$

(3) Vibrational mean free energy F :

$$F(\beta) = -kT \ln Z_{vib}(\beta) = -\frac{1}{\beta} \ln \left\{ e^{\beta \Lambda_3} \sqrt{\pi} \left[\frac{[1 - \text{Erf}(\Lambda_1 \sqrt{\beta})] - e^{\Lambda_4 \beta} [1 - \text{Erf}(\Lambda_2 \sqrt{\beta})]}{\Lambda_5 \sqrt{\beta}} \right] \right\}.\quad (29)$$

(4) Vibrational entropy S :

$$\begin{aligned}S(\beta) &= k \ln Z_{vib}(\beta) + kT \frac{\partial}{\partial T} \ln Z_{vib}(\beta) \\ &= k \left\{ \log \left[\frac{e^{\beta \Lambda_3} \sqrt{\pi} (\text{Erfc}(\sqrt{\beta} \Lambda_1) - e^{\beta \Lambda_4} \text{Erfc}(\sqrt{\beta} \Lambda_2))}{\Lambda_5 \sqrt{\beta}} \right] \right. \\ &\quad + \frac{\sqrt{\pi} ((1 - 2\beta \Lambda_3) \text{Erfc}(\sqrt{\beta} \Lambda_1) + e^{\beta \Lambda_4} (-1 + 2\beta(\Lambda_3 + \Lambda_4)) \text{Erfc}(\sqrt{\beta} \Lambda_2))}{2\sqrt{\pi} [\text{Erfc}(\sqrt{\beta} \Lambda_1) - e^{\beta \Lambda_4} \text{Erfc}(\sqrt{\beta} \Lambda_2)]} \\ &\quad \left. - \frac{e^{-\beta(\Lambda_1^2 + \Lambda_2^2)} \sqrt{\beta} (-e^{\beta \Lambda_2^2} \Lambda_1 + e^{\beta(\Lambda_1^2 + \Lambda_4)} \Lambda_2)}{\sqrt{\pi} [\text{Erfc}(\sqrt{\beta} \Lambda_1) - e^{\beta \Lambda_4} \text{Erfc}(\sqrt{\beta} \Lambda_2)]} \right\}.\end{aligned}\quad (30)$$

Table 1. Comparison of energy eigenvalues (in eV) obtained by using AIM with other methods for $2p$, $3p$, $3d$, $4d$, $4f$, $5p$, $5d$, $5f$, $5g$, $6p$, $6d$, $6f$ and $6g$ states in atomic units ($\hbar = m = 1$) for $r_e = 0.4$ and special case $D_1 = 15$, $D_2 = 0$.

states	a	Present	Exact [6]	Approximate [6]	LXC [43]	Local truncation error
$2p$	0.05	7.860804467	7.862800	7.86060	7.86080	0.0000044
	0.10	7.953304350	7.955370	7.95247	7.95330	0.0000041
	0.15	8.045099635	8.047240	8.04322	8.04510	0.0000009
	0.20	8.136203356	8.138420	8.13287	8.13620	0.0000024
	0.25	8.226628516	8.228920	8.22142	8.22663	0.0000030
	0.30	8.316388092	8.318740	8.30889	8.31639	0.0000041
$3p$	0.05	10.99776302	10.99980	10.9976	10.9978	0.0000370
	0.10	11.16256036	11.16470	11.1617	11.1626	0.0000400
	0.15	11.32424848	11.32647	11.3224	11.3242	0.0000480
	0.20	11.48283721	11.48513	11.4795	11.4828	0.0000360
	0.25	11.63833602	11.64068	11.6331	11.6383	0.0000340
	0.30	11.79075408	11.67565	11.7833	11.7908	0.0000480
$3d$	0.05	10.21598019	10.21651	10.2154	10.21598	0.0000200
	0.10	10.35353916	10.35409	10.3510	10.35353	0.0000380
	0.15	10.48935369	10.48992	10.4837	10.48935	0.0000480
	0.20	10.62346249	10.62403	10.6135	10.62346	0.0000400
	0.25	10.75590446	10.75645	10.7403	10.75591	0.0000000
	0.30	10.88671869	10.88719	10.8642	10.88672	0.0000120
$4p$	0.05	12.49760240	12.49920	12.4974	12.49760	0.0000020
	0.10	12.69679594	12.69851	12.6960	12.69680	0.0000040
	0.15	12.88834790	12.89010	12.8865	12.88835	0.0000470
	0.20	13.07224420	13.07400	13.0689	13.07224	0.0000430
	0.25	13.24846979	13.25010	13.2433	13.24847	0.0000320
	0.05	12.09829019	12.09890	12.0977	12.09829	0.0000100
$4d$	0.10	12.28500910	12.28570	12.2825	12.28501	0.0000080
	0.15	12.46641867	12.46715	12.4608	12.46642	0.0000170
	0.20	12.64256631	12.64324	12.6326	12.64257	0.0000370
	0.05	11.82078608	11.82090	11.8195	11.82079	0.0000140
	0.10	11.99796058	11.99810	11.9930	11.99796	0.0000410
	0.15	12.17169520	12.17180	12.1604	12.17170	0.0000080
$5p$	0.20	12.34206967	12.34210	12.3221	12.34207	0.0000360
	0.10	13.54214240	13.54340	13.5413	13.54214	0.0000420
	0.20	13.92898591	13.93010	13.9257	13.92999	0.0000150
$5d$	0.10	13.30679659	13.30750	13.3043	13.30680	0.0000040
	0.20	13.69266270	13.69310	13.6827	13.69266	0.0000400
	0.10	13.14759709	13.14780	13.1426	13.14760	0.0000040
$5f$	0.20	13.53343975	13.53330	13.5134	13.53344	0.0000340
	0.10	13.03797516	13.03790	13.0296	13.03798	0.0000270
	0.20	13.42710850	13.42667	13.3938	13.42711	0.0000010
$6p$	0.10	14.05208850	14.05300	14.0513	14.05209	0.0000120
	0.10	13.90704815	13.90750	13.9045	13.90705	0.0000470
$6d$	0.10	13.81118932	13.81130	13.8062	13.81119	0.0000120
	0.10	13.74661179	13.74660	13.7383	13.74361	0.0000090

4. Numerical results

We have calculated the vibrational–rotational bound-state energies of the Deng–Fan potential ($D_2 = 0$) for various n and ℓ quantum numbers with two different values of parameter r_e . In order to show the accuracy of our method, we have obtained the local truncation error ($E_{AIM} - E_{exact}$) for our calculations. As can be seen from the results presented in Tables 1 and 2, AIM results are very close to the exact values and there is excellent agreement with other methods found in the literature for short potential range. However, the difference between them is noticed for long potential

range. This implies that Equation (8) is not a good approximation for a centrifugal term when the potential parameter a becomes large.

In addition, the known spectroscopic values in Table 3 are used to obtain the energy states of a few selected diatomic molecules for various vibrational n and rotational ℓ angular momentum as shown in Tables 4–7. The criteria for the selection of these molecules are mainly due to the purposes that they serve in various aspect of physical, chemical and related studies [27,31–35]. These selected diatomic molecules are: H_2 , I_2 , CO ,

Table 2. Comparison of energy eigenvalues (in eV) obtained by using AIM with other methods for $2p$, $3p$, $3d$, $4d$, $4f$, $5p$, $5d$, $5f$, $5g$, $6p$, $6d$, $6f$ and $6g$ states in atomic units ($\hbar = m = 1$) for $r_e = 0.8$ and special case $D_1 = 15$, $D_2 = 0$.

states	a	Present	Exact [6]	Approximate [6]	LXC [43]	Local truncation error
$2p$	0.05	4.140887237	4.14208	4.14068	4.140887	0.0011928
	0.10	4.219180023	4.22040	4.21835	4.219180	0.0012202
	0.15	4.297392964	4.29870	4.29552	4.297393	0.0013076
	0.20	4.375546092	4.37690	4.37221	4.375547	0.0013549
	0.25	4.453659003	4.45510	4.44845	4.453660	0.0014425
	0.30	4.531750853	4.53320	4.52425	4.531752	0.0014513
$3p$	0.05	7.532791535	7.53500	7.53258	7.532792	0.0022085
	0.10	7.724764169	7.72710	7.72393	7.724764	0.0023361
	0.15	7.915178421	7.91770	7.91330	7.915179	0.0025221
	0.20	8.104040211	8.10660	8.10071	8.104041	0.0025608
	0.25	8.291353518	8.29410	8.28615	8.291354	0.0027480
	0.30	8.477120373	8.47990	8.46962	8.477121	0.0027818
$3d$	0.05	5.739751150	5.74040	5.73913	5.739751	0.0006490
	0.10	5.845769968	5.84650	5.84327	5.845770	0.0007308
	0.15	5.950677430	5.95150	5.94505	5.950678	0.0008242
	0.20	6.054532348	6.05530	6.04453	6.054534	0.0007706
	0.25	6.157393368	6.15820	6.14177	6.157395	0.0008112
	0.30	6.259318933	6.26010	6.23682	6.259322	0.0007876
$4p$	0.05	9.613013061	9.61560	9.61280	9.613013	0.0025870
	0.10	9.883523594	9.88620	9.88269	9.883524	0.0026766
	0.15	10.14855549	10.1514	10.1467	10.14856	0.0028450
	0.20	10.40805734	10.4111	10.4047	10.40806	0.0030440
	0.25	10.66197323	10.6650	10.6568	10.66197	0.0030280
	0.30	10.91322333	10.9161	10.9099	10.91322	0.0028780
$4d$	0.05	8.493343408	8.49480	8.49272	8.493344	0.0014568
	0.10	8.707110672	8.70870	8.70461	8.707111	0.0015901
	0.15	8.917806896	8.91940	8.91218	8.917808	0.0015947
	0.20	9.125503844	9.12720	9.11551	9.125505	0.0016991
	0.25	9.3334705654	9.33510	9.32346	9.333470	0.0003947
	0.30	9.541818181	9.54350	9.53142	9.541819	0.0003833
$4f$	0.05	7.735730867	7.73610	7.72448	7.735732	0.0003724
	0.10	7.882755012	7.88310	7.86276	7.882758	0.0003508
	0.15	11.30207233	11.3047	11.3012	11.30207	0.0026280
	0.20	11.91322333	11.9161	11.9099	11.91322	0.0028780
	0.25	10.52008576	10.5219	10.5176	10.52009	0.0018150
	0.30	11.06937036	11.0713	11.0594	11.06937	0.0019330
$5p$	0.05	9.796657408	9.79750	9.79166	9.796658	0.0008440
	0.10	10.27303457	10.2738	10.2530	10.27304	0.0007710
	0.15	9.152222313	9.15240	9.14389	9.152223	0.0001801
	0.20	9.552865312	9.55280	9.51954	9.552869	0.0000556
	0.25	12.27979911	12.2822	12.2790	12.27980	0.0024010
	0.30	11.73643833	11.7383	11.7339	11.73644	0.0018620
$5d$	0.05	11.24481430	11.2459	11.2398	11.24481	0.0010870
	0.10	10.81533124	10.8158	10.8070	10.81533	0.0004710
	0.15					
	0.20					
	0.25					
	0.30					
$5f$	0.05					
	0.10					
	0.15					
	0.20					
	0.25					
	0.30					
$5g$	0.05					
	0.10					
	0.15					
	0.20					
	0.25					
	0.30					
$6p$	0.05					
	0.10					
	0.15					
	0.20					
	0.25					
	0.30					
$6d$	0.05					
	0.10					
	0.15					
	0.20					
	0.25					
	0.30					
$6f$	0.05					
	0.10					
	0.15					
	0.20					
	0.25					
	0.30					
$6g$	0.05					
	0.10					
	0.15					
	0.20					
	0.25					
	0.30					

Table 3. Spectroscopic constants of the diatomic molecules studied in the present work.

Molecules	$D_1 = D_2 = D_e(eV)$	$r_e(A^\circ)$	$a(A^\circ^{-1})$	$\mu(amu)$	Molecules	$D_1 = D_2 = D_e(eV)$	$r_e(A^\circ)$	$a(A^\circ^{-1})$	$\mu(amu)$
<i>HCl</i>	4.619030905	1.2746	1.8677	0.9801045	<i>CrH</i>	2.13	1.694	1.52179	0.988976
<i>LiH</i>	2.5152672118	1.5956	1.1280	0.8801221	<i>NiC</i>	2.76	1.621	2.25297	9.974265
<i>H₂</i>	4.7446	0.7416	1.9426	0.50391	<i>CuLi</i>	1.74	2.310	1.00818	6.259494
<i>ScH</i>	2.25	1.776	1.41113	0.986040	<i>TiC</i>	2.66	1.790	1.52550	9.606079
<i>ScN</i>	4.56	1.768	1.50680	10.682771	<i>ScF</i>	5.85	1.794	1.46102	13.358942
<i>TiH</i>	2.05	1.781	1.32408	0.987371	<i>CO</i>	11.2256	1.1283	2.2994	6.8606719
<i>VH</i>	2.33	1.719	1.44370	0.988005	<i>I₂</i>	1.5556	2.662	1.8643	63.45223502

Table 4. Comparison of energy eigenvalues ($-E_{n\ell}$) for H_2 and LiH molecules (in eV) obtained by using AIM with the N-U method and the results obtained for Morse oscillator potential.

n	ℓ	H_2				LiH			
		Present	Morse [37,38]	N-U[10]	AP[10]	Present	Morse [37,38]	N-U[10]	AP[10]
0	0	4.394619779	4.47601	4.39444	4.39444	2.411949045	2.42886	2.41195	2.41195
	5	4.176618048	4.25880	4.17644	4.18054	2.383476249	2.40133	2.38348	2.38458
	10	3.621838424	3.72194	3.62165	3.63782	2.308147473	2.32884	2.30815	2.31229
5	0	1.758451567	2.22052	1.75835	1.75835	1.516277294	1.64771	1.51628	1.51628
	5	1.617410615	2.04355	1.61731	1.62548	1.492771433	1.62377	1.49278	1.49429
	10	1.260451640	1.60391	1.26034	1.29257	1.430614300	1.56074	1.43062	1.43627
7	0	1.077636993	1.53744	1.07756	1.07756	1.223393538	1.37756	1.22340	1.22340
	5	0.961814782	1.37656	0.96174	0.97232	1.201724343	1.35505	1.20173	1.20344
	10	0.669844065	0.97581	0.66976	0.71172	1.144438594	1.29580	1.14444	1.15083

Table 5. Comparison of energy eigenvalues ($-E_{n\ell}$) for CO and HCL molecules (in eV) obtained by using AIM with the N-U method and the results obtained for Morse oscillator potential.

n	ℓ	CO				HCL			
		Present	Morse [37,38]	N-U[10]	AP[10]	Present	Morse [37,38]	N-U[10]	AP[10]
0	0	11.08075178	11.0915	11.08068	11.08068	4.417077001	4.43556	4.41705	4.41705
	5	11.07253985	11.0844	11.07247	11.07354	4.374065784	4.39682	4.37403	4.37843
	10	11.05064581	11.0653	11.05057	11.05449	4.259761948	4.29408	4.25973	4.27591
5	0	9.688146187	9.79518	9.68809	9.68809	2.665748019	2.80506	2.66574	2.66574
	5	9.680226284	9.78833	9.68017	9.68130	2.628601192	2.77209	2.62859	2.63411
	10	9.659110919	9.77009	9.65905	9.66321	2.529905688	2.68471	2.52989	2.55027
7	0	9.159164003	9.29918	9.15911	9.15911	2.096524802	2.25701	2.09552	2.09652
	5	9.151359661	9.29246	9.15131	9.15247	2.061620020	2.22634	2.06961	2.06768
	10	9.130552425	9.27455	9.13050	9.13476	1.968892038	2.14511	1.96888	1.99127

Table 6. Energy spectra ($-E_{n\ell}$) (in eV) for ScH , ScN , TiH , VH and CrH molecules (in eV) for different values of the vibrational n and rotational ℓ quantum numbers.

n	ℓ	ScH	ScN	TiH	VH	CrH
0	0	2.1451493060	4.5117513960	1.9548048650	2.2469068330	2.0209482400
	5	2.1226840150	4.5095744780	1.9330370290	2.2331590720	1.9960456280
	10	2.0629653710	4.5037700670	1.8752225720	2.1965684350	1.9298629140
5	0	1.2437986870	4.044494640	1.1374524020	1.5053874500	1.0978208210
	5	1.2243617190	4.0423332560	1.1188747930	1.4930823830	1.0764456440
	10	1.1727049540	4.0366907290	1.0695483180	1.4603349300	1.0196528240
7	0	0.9554367725	3.8651682620	0.8761380413	1.2529130940	0.8106626600
	5	0.9371610441	3.8630761400	0.8587753818	1.2411662150	0.7906390670
	10	0.8885957808	3.8574978370	0.8126815790	1.2099057370	0.7374442293

Table 7. Energy spectra ($-E_{n\ell}$) (in eV) for NiC , $CuLi$, TiC , ScF and I_2 molecules (in eV) for different values of the vibrational n and rotational ℓ quantum numbers.

n	ℓ	NiC	$CuLi$	TiC	ScF	I_2
0	0	2.704655638	1.713181403	2.620886707	5.802429783	1.542189775
	5	2.701133597	1.711126336	2.618497121	5.800751287	1.541879340
	10	2.691742198	1.705648657	2.612126227	5.796275643	1.541051513
5	0	2.182832761	1.457654535	2.246784730	5.338269392	1.411303767
	5	2.179400530	1.455702193	2.244483737	5.336627904	1.410994391
	10	2.170248614	1.450498376	2.238349066	5.332250943	1.410169388
7	0	1.990100239	1.361759365	2.105700841	5.158417564	1.360584943
	5	1.986703730	1.359847420	2.103434910	5.156790781	1.360275990
	10	1.977647072	1.354751296	2.097393728	5.152453033	1.359452116

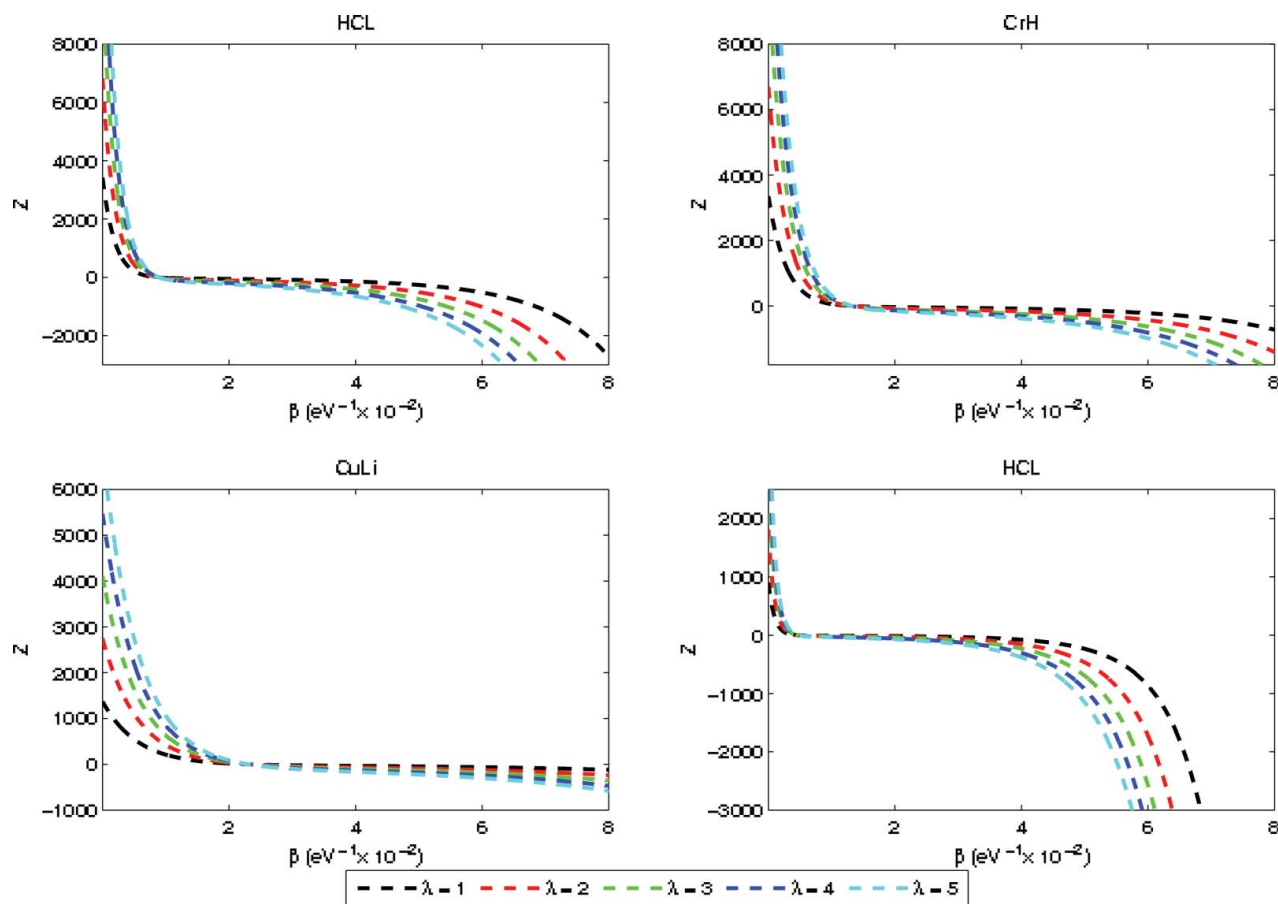


Figure 2. Vibrational partition function Z of HCl, CrH, CuLi and ScF diatomic molecules as a function of β for different λ .

HCl, LiH, ScH, TiH, VH, CrH, CuLi, TiC, NiC, ScN and ScF.

The spectroscopic parameters are taken from [10,27,34–41], also, the following conversion $1\text{amu} = 931.494028\text{MeV}/c^2$ [10,37] and $\hbar c = 1973.29\text{eV}\text{\AA}$ [10,35,37,38,42] are used throughout these calculations. We compare our numerical results with the few ones (H_2 , LiH, CO and HCL) that are available in the literature [10,37]. The rovibrational energies $-E_{n\ell}$ for H_2 , LiH, CO and HCL molecules (in eV) obtained by the present method (AIM) are compared with the Nikiforv–Uvarov (N–U) method [10], amplitude phase method (AP) [10] and the results obtained for Morse oscillator potential [10,37,38].

We have also studied the thermodynamic properties of this potential. We first obtained a high temperature partition function and then obtained thermodynamic functions, such as vibrational mean energy U , specific heat C , free energy F and entropy S with the application to some well-known diatomic molecules. From the variation of the thermodynamic properties obtained, we found that in Figure 2, for all the diatomic molecules Z monotonically decreases with λ and reaches a constant value for some typical values of λ

and then continues to decrease. In Figure 3, it is seen that Z monotonically increases with increasing λ . This is observed for all molecules except for ScF where Z decreases monotonically initially but finally rises.

In Figure 4, we found that U monotonically decreases with β until $\Delta\lambda \approx 0$. However in Figure 5, U increases with λ to the maximum value and then decreases with λ increasing, except for CuLi and ScF that only increases monotonically. As shown in Figure 6, C of all the molecules increases and decreases with some values of λ as β increases. On the other hand, in Figure 7, C first increases with λ to the maximum value and then remains constant and then finally increases with λ .

We observed that in Figure 8, F of HCl and ScF increases and decreases monotonically with β for some λ values but only decreases monotonically with β in the case of CuLi and ScF. However in Figure 9, F increases with λ to the maximum value and then decreases with λ increasing, except for ScF where no decrement was observed throughout the variation. As shown in Figure 10, S of HCl and CrF initially decrease with β and finally increases monotonically with increasing β . In the case of CuLi and ScF,

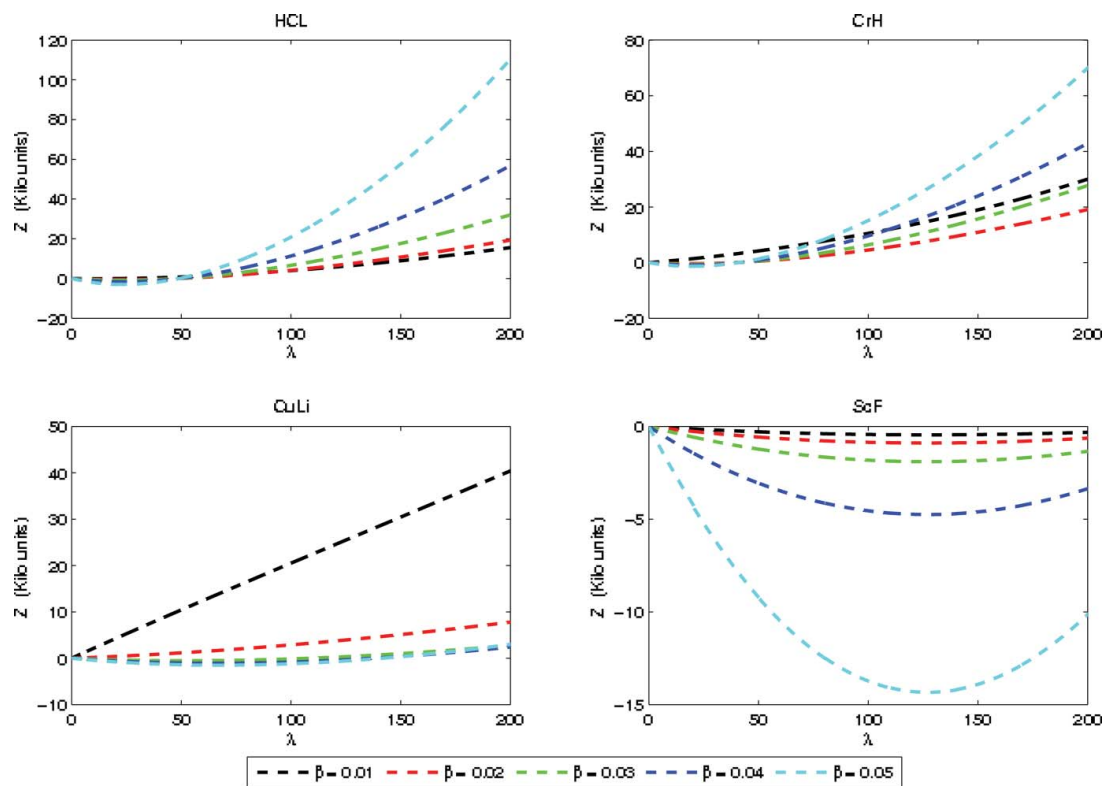


Figure 3. Vibrational partition function Z of HCl, CrH, CuLi and ScF diatomic molecules as a function of λ for different β .

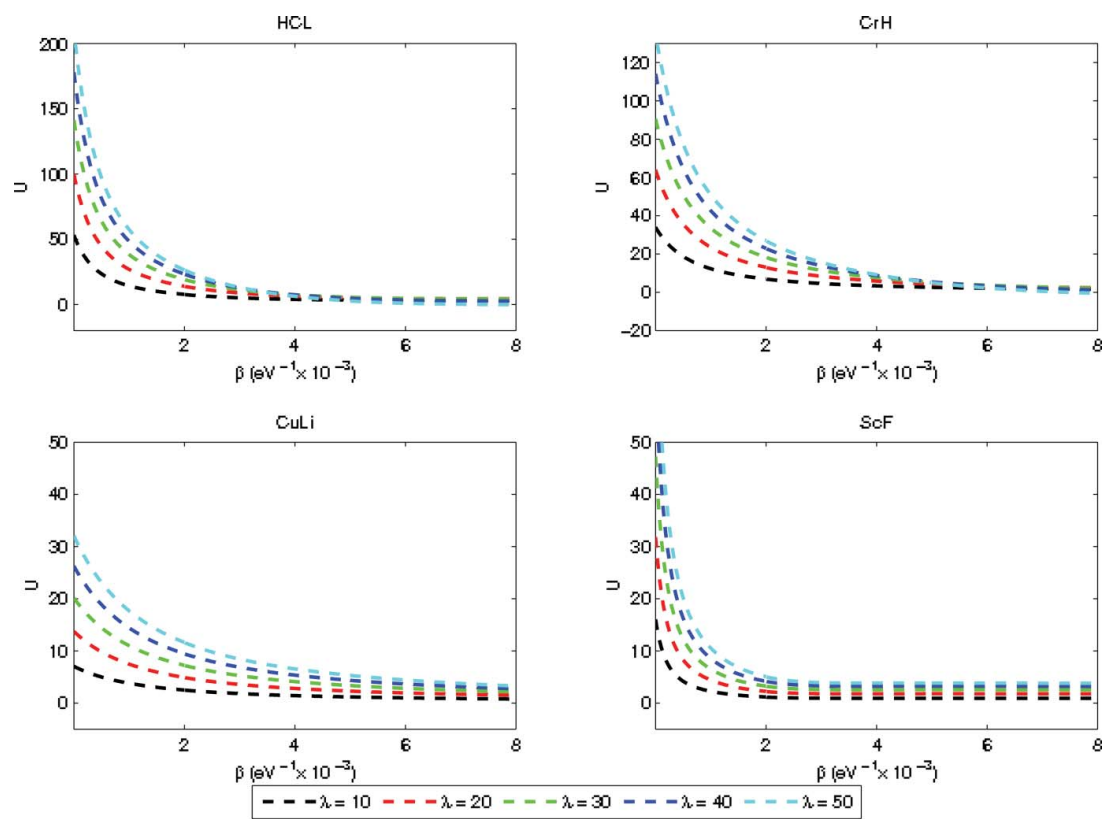


Figure 4. Vibrational mean energy U of HCl, CrH, CuLi and ScF diatomic molecules as a function of β for different λ .

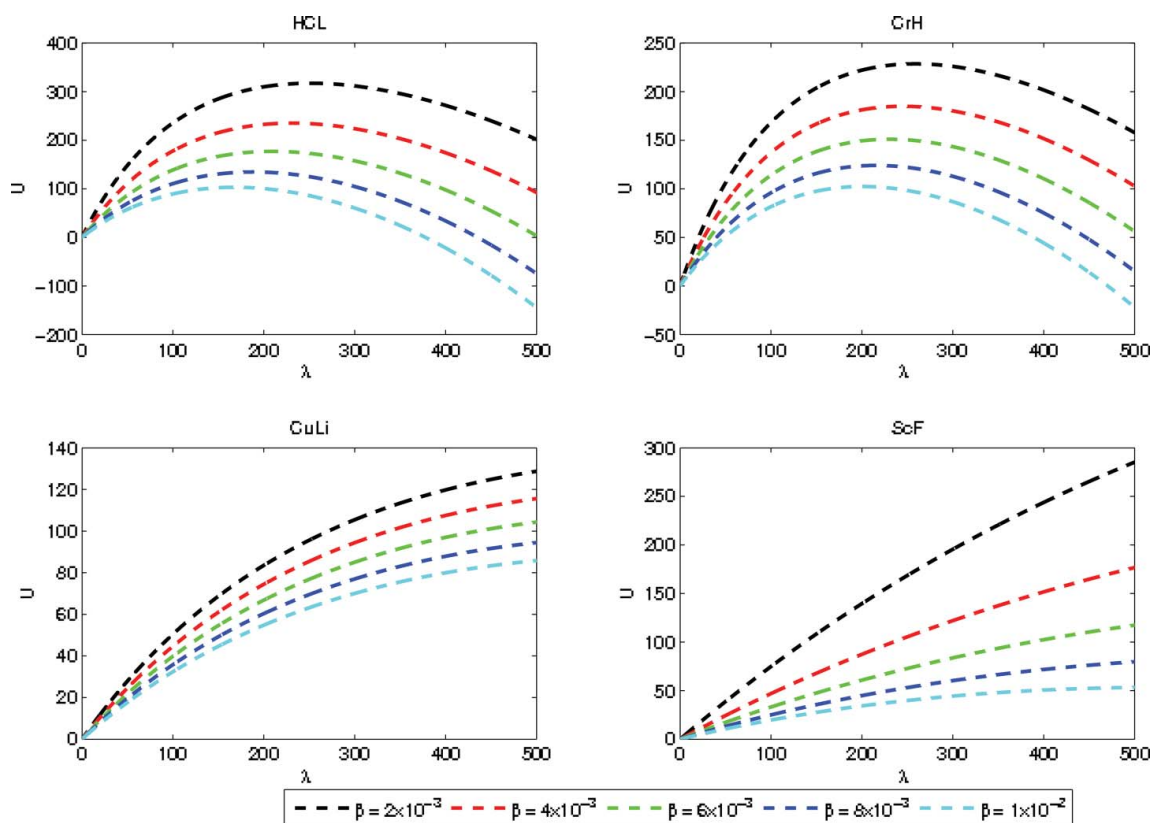


Figure 5. Vibrational mean energy U of HCl, CrH, CuLi and ScF diatomic molecules as a function of λ for different β .

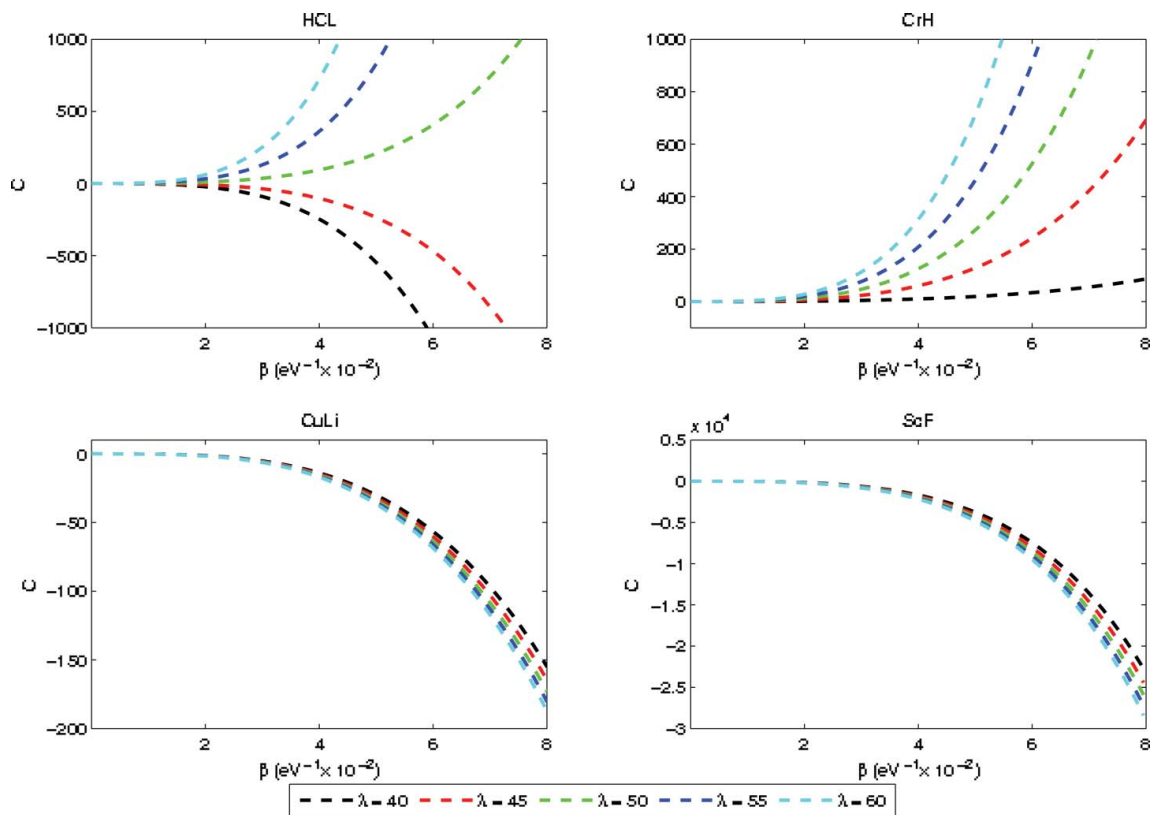


Figure 6. Vibrational free energy C of HCl, CrH, CuLi and ScF diatomic molecules as a function of β for different λ .

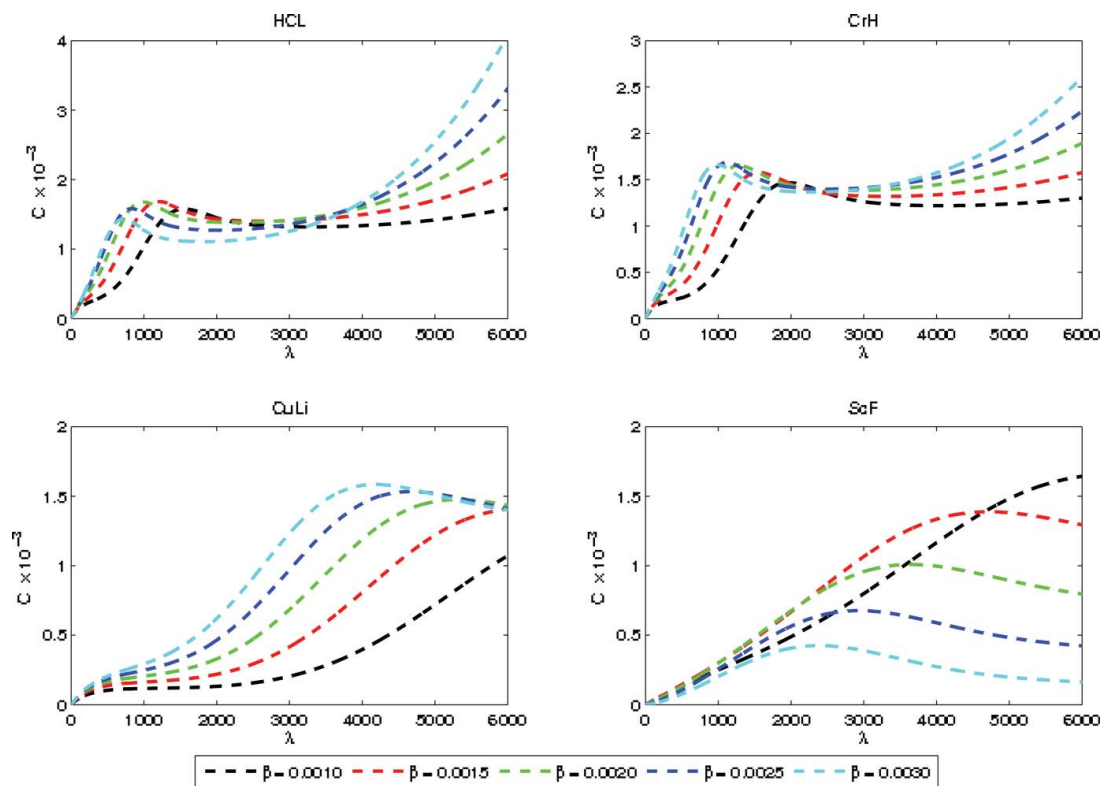


Figure 7. Vibrational free energy C of HCl, CrH, CuLi and ScF diatomic molecules as a function of λ for different β .

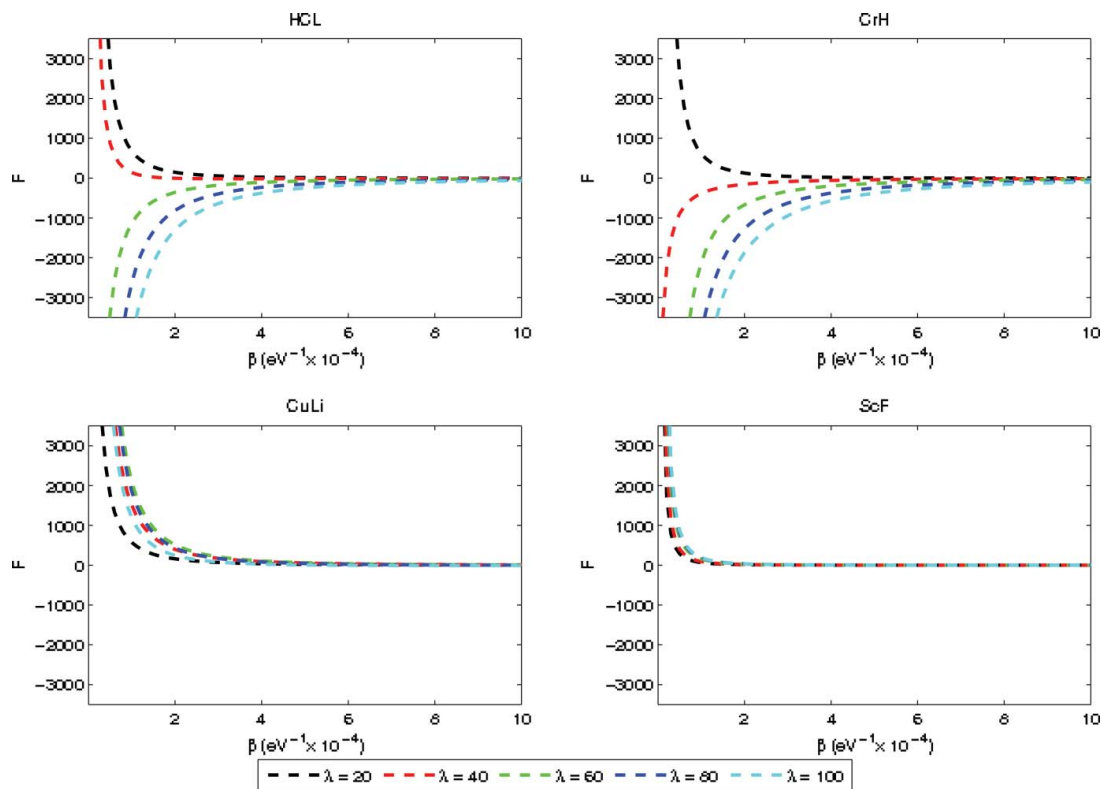


Figure 8. Vibrational free energy F of HCl, CrH, CuLi and ScF diatomic molecules as a function of β for different λ .

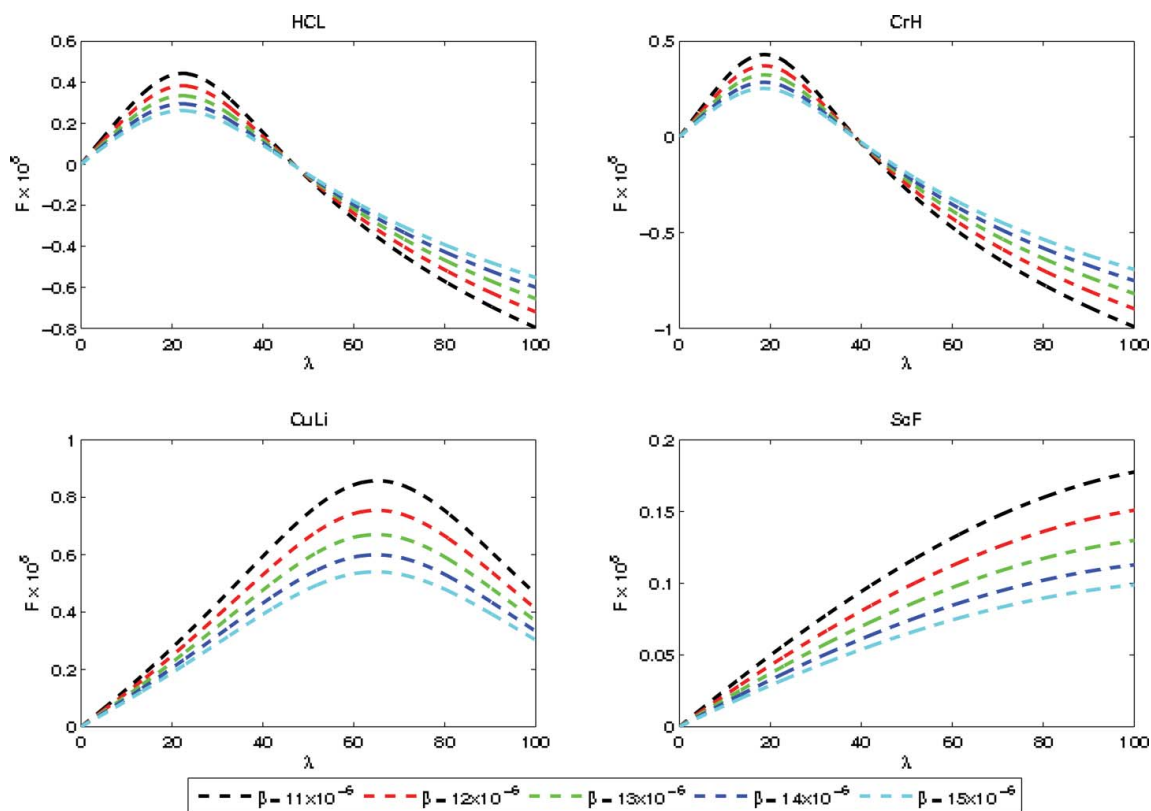


Figure 9. Vibrational free energy C of HCl, CrH, CuLi and ScF diatomic molecules as a function of λ for different β .

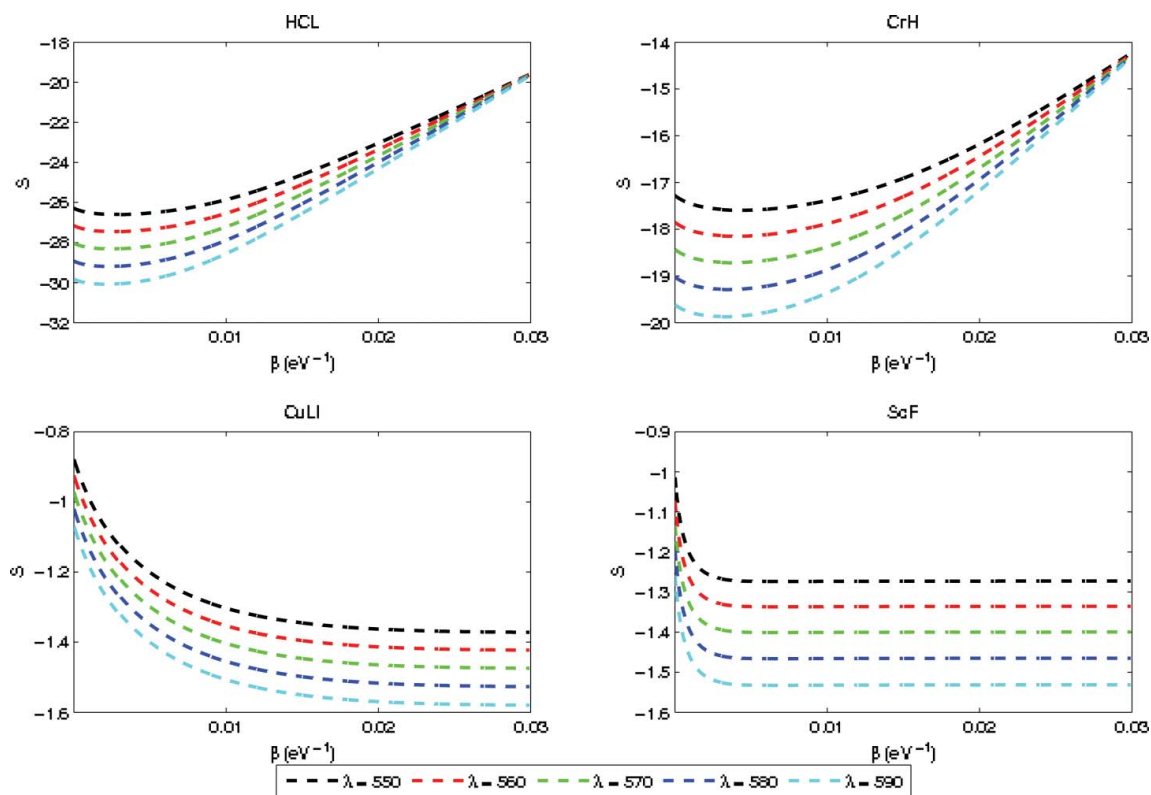


Figure 10. Vibrational free energy S of HCl, CrH, CuLi and ScF diatomic molecules as a function of β for different λ .

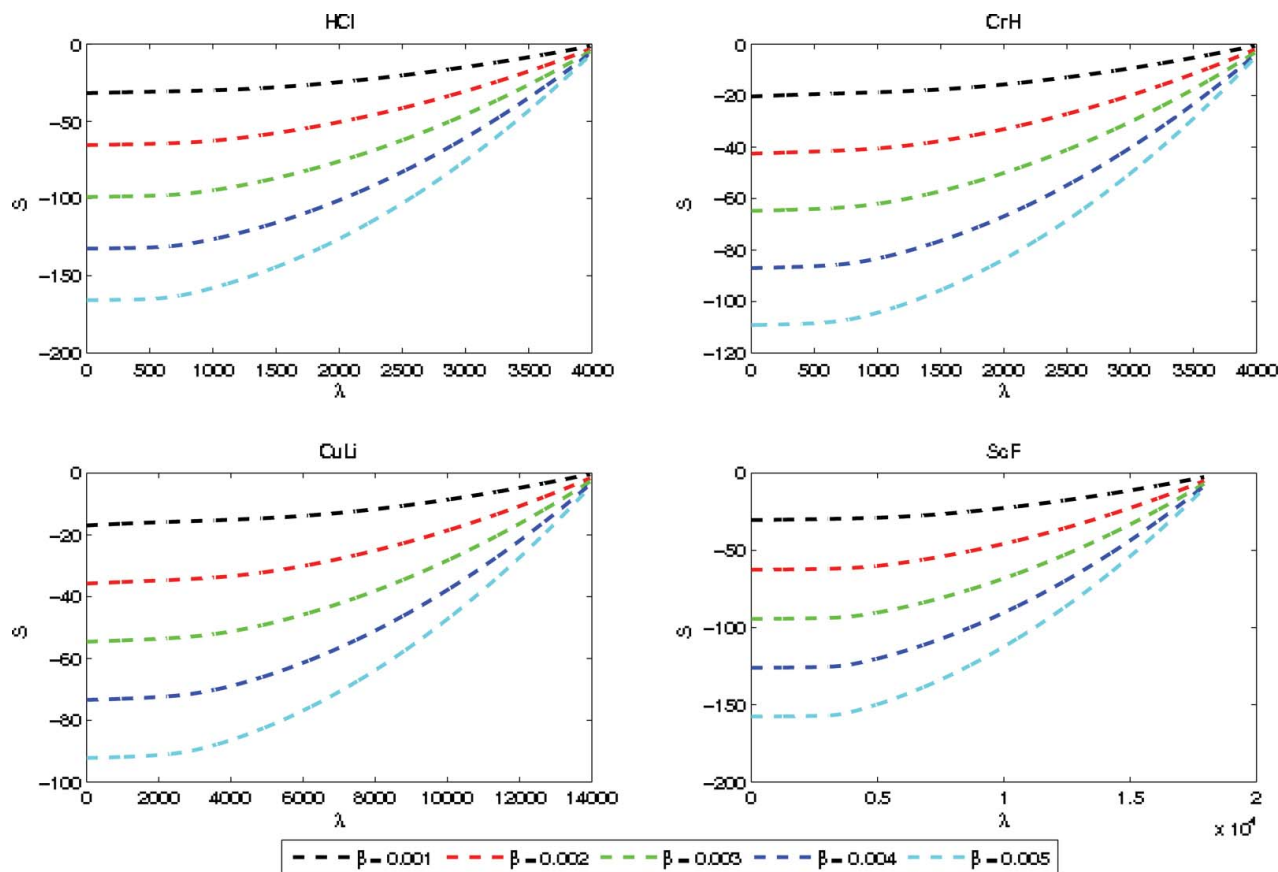


Figure 11. Vibrational free energy S of HCl, CrH, CuLi and ScF diatomic molecules as a function of λ for different β .

it decreases until it reaches a constant value. Finally, in Figure 11, it is shown that entropy S of each molecule for various β converge at a different range of λ .

5. Concluding remarks

In this study, we have solved the Schrödinger equation with the shifted Deng–Fan potential within the framework of the asymptotic iteration method. The energy eigenvalues and the corresponding normalised wave functions are obtained. In order to show the accuracy of our results, we have computed the eigenvalues numerically for arbitrary values of n and ℓ with two values of r_e for special case $D_2 = 0$ (Deng–Fan potential). A comparison of the present results with the ones obtained by Dong and Gu [6] and Zhang et al. [8], reveals that our results are accurate. It should be noted that, a similar investigation has been carried out on the Deng–Fan potential by Oyewumi et al. (2013) [36].

For $D_2 \neq 0$ (shifted Deng–Fan potential) that we have considered, the rovibrational energy levels for a few selected diatomic molecules have been presented. The results obtained are in excellent agreement with other results found in the literature; the Nikiforov–Uvarov (N–U) method and the amplitude phase method (AP). Also, the present results show that the shifted Deng–Fan and the Morse potentials are very close to each other, (see Tables 4 and 6).

Furthermore, we study the thermodynamic properties of this model potential. From a high temperature partition function obtained, thermodynamic functions, such as vibrational mean energy U , specific heat C , free energy F and entropy S are derived. It is found that in the classical limit, the vibrational entropy S converges to a point for all the diatomic molecules at a different range of β . Also, we have plotted the variation of some of these thermodynamic functions as a function of λ and β .

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