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Enthalpy, Gibbs free energy and specific heat in constant pressure for diatomic molecules using improved deformed exponential-type potential (IDEP)

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Abstract In this work, we have studied such thermal function of diatomic molecules like hydrogen dimer, carbon monoxide, nitrogen dimer and lithium hydride using improved deformed exponential-type potential (IDEP). To this end, the energy spectra of the IDEP are obtained applying Greene-Aldrich approximation and appropriate coordinate transformation within the framework of non-relativistic quantum mechanics. With calculated energy eigenstates, we have deduced the partition function and such thermodynamic functions like specific heat in constant pressure, enthalpy and Gibbs free energy by employing the Poisson summation formula. We have compared our results with experimental data, and there is a good agreement between them.

1 Introduction

In the past few years, predict and interpret the thermodynamic properties of the various system have been attendant by many scientists [1–6]. These properties like entropy, specific heat, mean energy, etc., are based on information about interaction potential [7–11]. According to industrial, we can see that accurate prediction of the properties has an important effect in physics, chemistry, engineering and material science [12–16]. Also, the properties have an important role in phase transition, adsorption and synthesis of materials [17–19].

In the last few decades, the analytical solution of wave equations for interaction potential models in quantum mechanics has been interested by many researchers. Therefore, one of the interesting ways of calculating the thermodynamic properties of systems is to know the interaction potential of them. So far, some potential models have been applied in literature such as Tietz-Wei, Deng-Fan, Hulthen, Morse, Manning-Rosen and Tietz [20–25]. By considering an interaction potential and solving Schrödinger equation (SE), one can obtain the energy spectrum and thereby partition function of a corresponding system.

It is well known that the accurate solution of SE for a potential model has an important effect on calculating thermodynamic properties. The exact solution of SE for the hydrogen atom and harmonic oscillator are two typical examples in quantum mechanics [26]. Luise et al. [27] obtained the approximation solutions of the SE with Manning-Rosen plus Hell-

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mann potential for any l-state by using the proper quantization rule. Oliveira et al. [28] exactly solve the SE written on a spherical surface and interacting with the Pöschl–Teller double ring shaped potential and calculated their energy eigenvalues. Udoh et al. [29] solved the SE for the improved Rosen-Morse potential model in D spatial dimensions by using the Nikiforov–Uvarov method. Also, they obtained the rotational-vibrational energies and the wave function. Badalov et al. [30] obtained the approximation analytical solutions of the hyper-radial SE for the generalized Wood-Saxon potential by using the Pekeris approximation.

The system of our interest is exponential-type potential function that has been studied by many authors [31–33]. Jia et al. [34] exactly solved the SE for a five-parameter exponential type model in two cases from first principles. Xie et al. [35] reported an improved multi-parameter exponential-type potential energy model for diatomic molecules. They showed that this potential is identical to the Tietz potential in the realm of diatomic molecules. In this work, we have solved the SE for IDEP by using the Greene-Aldrich approximation and obtained energy eigenvalues. Then we have determined partition function and thereby such thermodynamic properties of diatomic molecules such as H_2, CO, N_2 and LiH. We have compared our results with experimental data extracted from the National Institute of Standards and Technology (NIST) database [36].

2 Solution of SE with the IDEP

The time-independent radial SE is express as follow [37]

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2R_{nl}(r)}{\mathrm{d}r^2}+\left[V(r)+\frac{l(l+1)}{2\mu r^2}\right]R_{nl}(r)=E_{nl}R_{nl}(r) \tag{1}$$

where μ is the reduced mass, E_{nl} is the energy spectrum of the IDEP to be determined, $\hbar$ is the Planck constant, and n and l are the vibrational and rotational quantum numbers, respectively. Here, the potential model to be employed is defined as

$$V_{\text{IDEP}}(r)=D_e\left(1-\frac{q-e^{2\alpha(r_e-r_0)}}{q-e^{2\alpha(r-r_0)}}\right)^2 \tag{2}$$

where D_e is the dissociation energy, r_e is the equilibrium bond length, and q, α and r_0 are parameters that can be expressed corresponds to the diatomic molecular constants with the following relations:

$$q=\left(1-\frac{\alpha}{\pi c\omega_e}\sqrt{\frac{2D_e}{\mu}}\right)e^{2\alpha(r_e-r_0)} \tag{3}$$

$$\alpha=3\pi c\omega_e\sqrt{\frac{\mu}{2D_e}}-\frac{16\pi^3c^2\mu^2r_e^3\omega_e\alpha_e}{3h^2}-\frac{1}{2\pi r_e} \tag{4}$$

$$r_0=r_e-\frac{1}{9\pi c\omega_e\sqrt{\frac{\mu}{2D_e}}-\frac{16\pi^3c^2\mu^2r_e^3\omega_e\alpha_e}{h^2}-\frac{3}{2\pi r_e}}\ln\left(\frac{32\pi^3c^2\mu^2r_e^4\omega_e^2\alpha_e+\frac{3h^2\omega_e}{\pi}}{3h^2+2\pi cr_e\omega_e}\right) \tag{5}$$

where ω_e is the equilibrium harmonic vibrational frequency, α_e is the vibrational rotation coupling constant, and c is the speed of light. It is clear that the IDEP reduces to Tietz potential by replacing 2α to α and $-qe^{2\alpha r_0}$ to $\hbar$ [2]. Substituting Eq. (2) into Eq. (1) and by considering Eqs. (3)–(5), the following results has been obtained

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2 R_{nl}(r)}{\mathrm{d}r^2}+\left[D_e\left(1-\frac{q-e^{2\alpha(r_e-r_0)}}{q-e^{2\alpha(r-r_0)}}\right)^2+\frac{l(l+1)}{2\mu r^2}\right]R_{nl}(r)=E_{nl}R_{nl}(r) \tag{6}$$

Due to the presence of the centrifugal term $\frac{l(l+1)}{r^2}$, we cannot solve Eq. (6) for the case $l \neq 0$ analytically. Therefore, we use the improved Greene-Aldrich approximation to deal with the centrifugal term to remove this problem. This approximation is written as [38]

$$\frac{1}{r^2}=4\alpha^2\left(d_0+\frac{e^{2\alpha r}}{\left(Q-e^{2\alpha r}\right)^2}\right),\quad d_0=\frac{1}{2} \tag{7}$$

Substituting Eq. (7) into Eq. (6) and Applying the coordinate transformation $= e^{2\alpha r}$, the following yields

$$s^2\frac{\mathrm{d}^2 R_{nl}(s)}{\mathrm{d}s^2}+s\frac{\mathrm{d}R_{nl}(s)}{\mathrm{d}s}+\left[-\varepsilon_{nl}+\frac{A}{(Q-s)}+\frac{B-\gamma s}{(Q-s)^2}\right]R_{nl}(s)=0 \tag{8}$$

where $Q = qe^{2\alpha r_0}$ and $\gamma = l(l+1)$. Here, we use the following abbreviations

$$\begin{aligned}
\varepsilon_{nl}&=-\left[\frac{1}{4\hbar^2\alpha^2}\left(2\mu E_{nl}-4\gamma\hbar^2\alpha^2 d_0-2\mu D_0\right)\right];\\
A&=\frac{\mu D_e}{\hbar^2\alpha^2}\left(Q-e^{2\alpha r_e}\right);\\
B&=-\frac{\mu D_e}{\hbar^2\alpha^2}\left(Q-e^{2\alpha r_e}\right)^2.
\end{aligned} \tag{9}$$

We suppose that the wave function has the form $R_{nl}(s) = s(Q-s)^{\delta}F_{nl}(s)$. Therefore, by some mathematical computation, the following equation has been obtained

$$\begin{aligned}
s(Q-s)\frac{\mathrm{d}^2 F_{nl}(s)}{\mathrm{d}F^2}&+[Q(1+2)-(1+2+2\delta)s]\frac{\mathrm{d}F_{nl}(s)}{\mathrm{d}F}\\
&-\left[\left(+\delta-\sqrt{\varepsilon_{nl}}\right)\left(+\delta-\sqrt{\varepsilon_{nl}}\right)\right]F_{nl}(s)=0
\end{aligned} \tag{10}$$

where

$$\eta=\pm\sqrt{\varepsilon_{nl}-\left(\frac{A}{Q}+\frac{B}{Q^2}\right)};\quad \delta=\frac{1}{2}\left(1\pm\sqrt{1-4\left(\frac{B}{Q^2}-\frac{\gamma}{Q}\right)}\right) \tag{11}$$

Equation (10) is a hypergeometric equation, and its solution is the hypergeometric function given in the form [6]

$$F_{nl}(s)=2F_1(a_1,b_1;c_1;s)=\frac{\Gamma(c_1)}{\Gamma(a_1)\Gamma(b_1)}=\sum_{t=0}^{\infty}\frac{\Gamma(a_1+t)\Gamma(b_1+t)}{\Gamma(c_1+t)}\frac{s^t}{t!} \tag{12}$$

where

$$\begin{aligned}
a_1&=+\delta-\sqrt{\varepsilon_{nl}};\\
b_1&=+\delta+\sqrt{\varepsilon_{nl}};\\
c_1&=Q(1+2).
\end{aligned} \tag{13}$$

We can see that when either a_1 or b_1 is equal to a negative integer $(-n)$, then the hypergeometric function $F_{nl}(s)$ will become a polynomial of a certain degree. This scheme leads the hypergeometric function to a finite one under the following quantum condition

$$a_1 = -n. \quad n = 0, 1, 2, 3, \ldots, n_{\max} \tag{14}$$

where

$$n_{\max} = \sqrt{\frac{\mu D_e\left(Q - e^{2\alpha r_e}\right)}{\hbar^2\alpha^2 Q}\left(1 - \frac{\left(Q - e^{2\alpha r_e}\right)}{2Q}\right)} - \frac{1}{2}\left(1 \pm \sqrt{\frac{(Q+2l)^2}{Q^2} + \frac{2\mu D_e\left(Q - e^{2\alpha r_e}\right)^2}{\hbar^2\alpha^2 Q^2}}\right) \tag{15}$$

Substituting Eqs. (10) and (11) into Eq. (13) and by some complex mathematical calculation, the following expression obtain

$$\varepsilon_{nl} = \left[\frac{(n+)}{2} + \frac{\xi}{2(n+\delta)}\right]^2 \tag{16}$$

where

$$\xi = \left(\frac{A}{Q} + \frac{B}{Q^2}\right) \tag{17}$$

Substituting Eqs. (9), (11) and (16) into Eq. (17), the energy spectra for the IDEP has been deduce as

$$E_{nl} = D_e + \frac{2\hbar^2\alpha^2}{\mu}\frac{l(l+1)}{12} - \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{2n+1 \pm \sqrt{\frac{(Q+2l)^2}{Q^2} + \frac{2\mu D_e\left(Q-e^{2\alpha r_e}\right)^2}{\hbar^2\alpha^2 Q^2}}}{4} + \frac{\frac{\mu D_e\left(Q-e^{2\alpha r_e}\right)}{\hbar^2\alpha^2 Q}\left(1 - \frac{\left(Q-e^{2\alpha r_e}\right)}{2Q}\right)}{2n+1 \pm \sqrt{\frac{(Q+2l)^2}{Q^2} + \frac{2\mu D_e\left(Q-e^{2\alpha r_e}\right)^2}{\hbar^2\alpha^2 Q^2}}}\right]^2 \tag{18}$$

In Eq. (18), plus and negative sign corresponds to $Q < 0$ and $Q > 0$, respectively. By considering $l = 0$, Eq. (18) reduces to the energy spectra for the IDEP which is identical to the pure energy levels represented by the improved Tietz potential function [6].

Table 1 Spectroscopic parameters for the selected diatomic molecules [39, 40]

Molecules	D_e (cm^{-1})	r_e (Å)	μ (amu)
H_2	38,297.00	0.7416	0.5039
CO	90,529.00	1.1283	6.8562
N_2	79,885.00	1.0970	7.0034
LiH	20,287.70	1.5955	0.8801

Table 2 Calculated values of the IDEP parameters for different diatomic molecules

Molecules	$\alpha \times 10^7$ (cm^{-1})	$r_0 \times 10^{-8}$ (cm)	q
H_2	25.73680374	0.741600148	– 0.3236073943
CO	30.69381001	1.128300118	– 0.6544806294
N_2	36.42844874	1.097000113	– 0.3543700921
LiH	15.02728120	1.595500403	– 0.3326882575

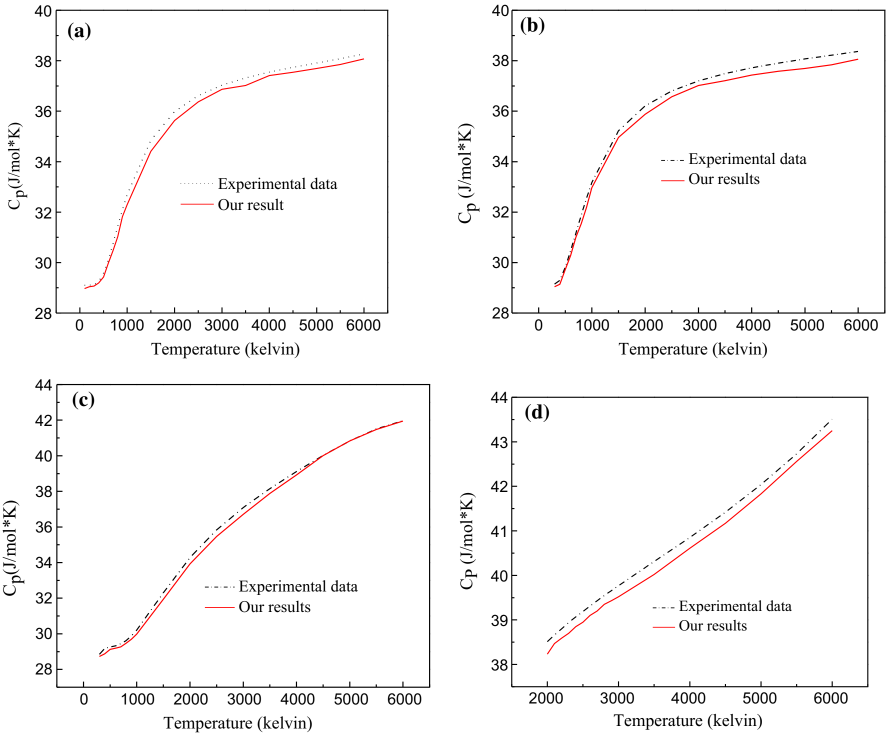

Fig. 1 Specific heat in constant pressure versus temperature for diatomic molecules: **a** N_2 with $\alpha = 36.42844874$, $r_0 = 1.097000113$ and $q = -0.3543700921$, **b** CO with $\alpha = 30.69381001$, $r_0 = 1.128300118$ and $q = -0.6544806294$, **c** H_2 with $\alpha = 25.73680374$, $r_0 = 0.7416001485$ and $q = -0.3236073943$, **d** LiH with $\alpha = 15.02728120$, $r_0 = 1.595500403$ and $q = -0.3326882575$

3 Thermodynamic function of the IDEP

The first point to determine thermodynamic function of a system is calculating partition function. The bound state contributions to the partition function of any system at a given temperature T is define as

$$Z(\beta, \lambda) = \sum_{n=0}^{\lambda} e^{-\beta E_{nl}}, \quad \beta = (k_B T)^{-1} \tag{19}$$

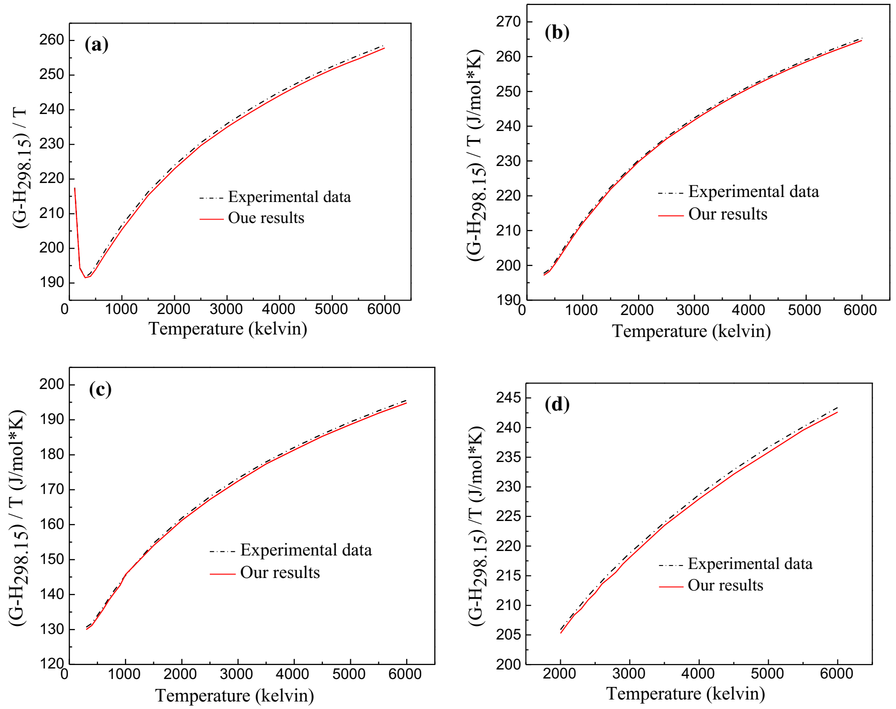

Fig. 2 Gibbs free energy versus temperature for diatomic molecules: **a** N_2 with $\alpha = 36.42844874$, $r_0 = 1.097000113$ and $q = -0.3543700921$, **b** CO with $\alpha = 30.69381001$, $r_0 = 1.128300118$ and $q = -0.6544806294$, **c** H_2 with $\alpha = 25.73680374$, $r_0 = 0.7416001485$ and $q = -0.3236073943$, **d** LiH with $\alpha = 15.02728120$, $r_0 = 1.595500403$ and $q = -0.3326882575$

where k_B is the Boltzmann constant, λ is the upper bound quantum number, and E_{nl} is the energy eigenvalues of IDEP. The pure energy levels can be written as

$$E_n = D_e - \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{\left(n+\frac{1}{2}\left(1\pm\sqrt{1+\frac{2\mu D_e\left(Q-e^{2\alpha r_e}\right)^2}{\hbar^2\alpha^2Q^2}}\right)\right)}{2}+\frac{\frac{\mu D_e\left(Q-e^{2\alpha r_e}\right)}{\hbar^2\alpha^2Q}\left(1-\frac{\left(Q-e^{2\alpha r_e}\right)}{2Q}\right)}{2\left(n+\frac{1}{2}\left(1\pm\sqrt{1+\frac{2\mu D_e\left(Q-e^{2\alpha r_e}\right)^2}{\hbar^2\alpha^2Q^2}}\right)\right)}\right]^2 \tag{20}$$

Substituting Eq. (20) into Eq. (19), the partition function deduce as follow

$$Z(\beta,\lambda) = \sum_{n=0}^{\lambda}\exp\left\{-\beta\left(D_e - \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{(n+\xi)}{2}+\frac{\zeta}{2(n+\xi)}\right]^2\right)\right\} \tag{21}$$

where

$$\zeta = \frac{\mu D_e\left(Q-e^{2\alpha r_e}\right)}{\hbar^2\alpha^2Q}\left(1-\frac{\left(Q-e^{2\alpha r_e}\right)}{2Q}\right) \tag{22}$$

$$\xi = \frac{1}{2}\left(1\pm\sqrt{1+\frac{2\mu D_e\left(Q-e^{2\alpha r_e}\right)^2}{\hbar^2\alpha^2Q^2}}\right) \tag{23}$$

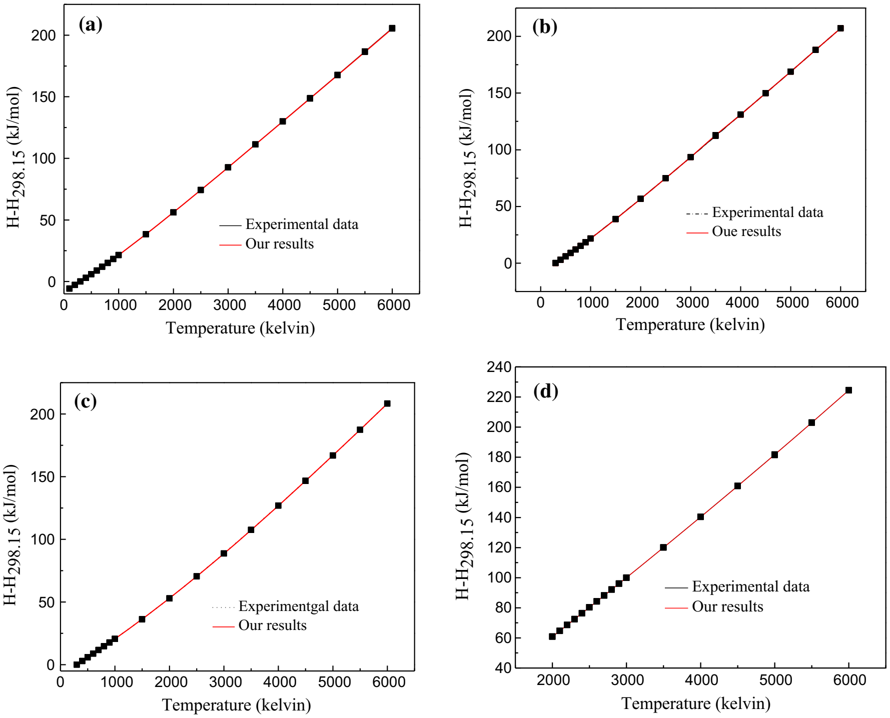

Fig. 3 Enthalpy versus temperature for diatomic molecules: **a** N_2 with $\alpha = 36.42844874$, $r_0 = 1.097000113$ and $q = -0.3543700921$, **b** CO with $\alpha = 30.69381001$, $r_0 = 1.128300118$ and $q = -0.6544806294$, **c** H_2 with $\alpha = 25.73680374$, $r_0 = 0.7416001485$ and $q = -0.3236073943$, **d** LiH with $\alpha = 15.02728120$, $r_0 = 1.595500403$ and $q = -0.3326882575$

To calculating Eq. (21), we use the Poisson summation formula for lower order approximation as

$$\sum_{n=0}^{n_{\max}} f(x) = \frac{1}{2}[f(0) - f(n_{\max}+1)] + \int_{0}^{n_{\max}+1} f(y)\mathrm{d}y \tag{24}$$

By substituting Eq. (21) into Eq. (24), one can obtain the following functions

$$\begin{aligned} f(0) &= \exp\left\{-\beta\left(D_e - \left(\frac{\hbar^2\alpha^2}{2\mu}\right)\left(\frac{\xi}{2} + \frac{\zeta}{2\xi}\right)^2\right)\right\}; \\ f(\lambda+1) &= \exp\left\{-\beta\left(D_e - \left(\frac{\hbar^2\alpha^2}{2\mu}\right)\left(\frac{(\lambda+1+\xi)}{2} + \frac{\zeta}{2(\lambda+1+\xi)}\right)^2\right)\right\}. \end{aligned} \tag{25}$$

Also

$$\int_{0}^{\lambda+1} f(x)\mathrm{d}x = \int_{0}^{\lambda+1} \exp\left\{-\beta\left(D_e - \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{(\lambda+1+\xi)}{2} + \frac{\zeta}{2(\lambda+1+\xi)}\right]^2\right)\right\}\mathrm{d}\lambda \tag{26}$$

By evaluating the integral part of the right-hand side of Eq. (26), we have

$$\int_{0}^{\lambda+1} f(x)\mathrm{d}x = \int_{G_1}^{G_2} \exp\{-\beta(D_e - H\rho^2)\}\left(1 + \frac{\rho}{\sqrt{\rho^2-\zeta}}\right)\mathrm{d}\rho \tag{27}$$

In the above integral, $G_1 \frac{\xi}{2} + \frac{\zeta}{2\xi}$ and $G_2 = \frac{(\lambda+1+\xi)}{2} + \frac{\zeta}{2(\lambda+1+\xi)}$. Here, we have define the parameter

$$\rho = \frac{(\lambda+1+\xi)}{2} + \frac{\zeta}{2(\lambda+1+\xi)} \tag{28}$$

By calculating Eq. (27) and combining with Eq. (25), the partition function of IDEP is obtained by employing Maple software as

$$\begin{aligned} Z(\beta,\lambda) = \frac{1}{2}e^{-\beta D_e}\Bigg\{ & e^{\beta H G_1^2} - e^{\beta H G_2^2} + \sqrt{\frac{\pi}{H\beta}}\Big[-\mathrm{erfi}\left(G_1\sqrt{H\beta}\right) - \mathrm{erfi}\left(G_2\sqrt{H\beta}\right) \\ & + e^{H\zeta\beta}\left(-\mathrm{erfi}\left(\sqrt{H\beta}\sqrt{G_1^2-\zeta}\right) + \mathrm{erfi}\left(\sqrt{H\beta}\sqrt{G_2^2-\zeta}\right)\right)\Big]\Bigg\} \end{aligned} \tag{29}$$

where the imaginary error function is defined as

$$\mathrm{erfi}(u) = \frac{\mathrm{erf}(iu)}{i} = \frac{2}{\sqrt{\pi}}\int_{0}^{u} e^{t^2}\mathrm{d}t \tag{30}$$

with the help of the vibrational partition function of Eq. (29), other thermodynamic functions of IDEP can be obtained using the following expressions:

- Internal energy

$$U(\beta,\lambda) = -\frac{\partial \ln Z(\beta,\lambda)}{\partial\beta} \tag{31}$$

- Entropy

$$S(\beta,\lambda) = k_{\mathrm{B}}\ln Z(\beta,\lambda) - k_{\mathrm{B}}\beta\frac{\partial \ln Z(\beta,\lambda)}{\partial\beta} \tag{32}$$

- Enthalpy

$$H(\beta,\lambda) = U(\beta,\lambda) + \mathrm{PV} \tag{33}$$

- Gibbs free energy

$$G(\beta,\lambda) = H(\beta,\lambda) - TS(\beta,\lambda) \tag{34}$$

- Specific Heat in constant pressure

$$c_P(\beta,\lambda) = -k_{\mathrm{B}}\beta^2\frac{\partial H(\beta,\lambda)}{\partial\beta} \tag{35}$$

4 Results and discussion

In this paper, we have considered the electronic states of diatomic molecules such as hydrogen dimer, carbon monoxide, nitrogen dimer and lithium hydride using energy spectra of Eq. (18). The experimental values of the selected diatomic molecules are given in Table 1 [39, 40]. Also,

Table 3 Specific heat in constant pressure deviations of N_2, CO, H_2 and LiH using the potential model

Temperature	N_2	CO	H_2	LiH
100	1.45			
200	1.41			
300	1.45	1.45	1.43	
400	1.46	1.46	1.44	1.92
500	1.47	1.49	1.45	1.93
600	1.50	1.52	1.45	1.94
700	1.53	1.55	1.46	1.94
800	1.57	1.59	1.47	1.95
900	1.6	1.62	1.48	1.95
1000	1.63	1.65	1.49	1.96
1500	1.74	1.76	1.59	1.97
2000	1.79	1.81	1.69	1.97
2500	1.83	1.84	1.77	1.98
3000	1.85	1.86	1.83	1.98
3500	1.86	1.87	1.89	2.01
4000	1.87	1.88	1.94	2.04
4500	1.87	1.89	2	2.07
5000	1.89	1.9	2.04	2.1
5500	1.9	1.91	2.07	2.13
6000	1.91	1.91	2.09	2.17

Table 4 Gibbs free energy deviations of N_2, CO, H_2 and LiH using the potential model

Temperature	N_2	CO	H_2	LiH
100	1.875			
200	1.715			
300	1.58	1.885	1.5	
400	1.64	1.94	1.55	1.26
500	1.745	1.05	1.675	1.342
600	1.87	1.17	1.78	1.41
700	1.99	1.295	1.914	1.71
800	1.11	1.415	1.02	1.54
900	1.225	1.53	1.129	1.60
1000	1.335	1.64	1.28	1.68
1500	1.815	1.125	1.70	1.72
2000	1.2	1.515	1.06	1.78
2500	1.525	1.845	1.36	1.84
3000	1.8	1.12	1.62	1.904
3500	1.04	1.365	1.86	1.17
4000	1.255	1.58	1.06	1.39
4500	1.45	1.775	1.26	1.6
5000	1.625	1.955	1.43	1.79
5500	1.785	1.115	1.59	1.97
6000	1.935	1.265	1.745	1.13

Table 5 Enthalpy deviations of N_2, CO, H_2 and LiH using the potential model

Temperature	N_2	CO	H_2	LiH
100	0.28			
200	0.14			
300	0.00	0.001	0.002	
400	0.14	0.14	0.14	3.04
500	0.29	0.29	0.29	3.23
600	0.44	0.44	0.44	3.43
700	0.59	0.59	0.58	3.62
800	0.75	0.75	0.73	3.81
900	0.91	0.91	0.88	4.01
1000	1	1.08	1.03	4.21
1500	1.92	1.94	1.81	4.4
2000	2.8	2.83	2.64	4.6
2500	2.71	2.74	2.52	4.81
3000	2.63	2.67	2.43	5
3500	2.56	2.64	3.38	5.005
4000	2.5	3.54	3.34	5.02
4500	2.44	3.49	3.33	5.04
5000	3.39	3.44	3.34	5.09
5500	3.34	4.39	3.37	5.15
6000	3.39	4.35	4.41	5.22

the values of the molecular parameters q, α and r_0 for the selected diatomic molecules are obtained using Eqs. (3)–(5), respectively. These values are tabulated in Table 2. Figure 1a–d show the specific heat in constant pressure for the diatomic molecules versus temperature at the range 100–6000 °K for nitrogen dimer, 300–6000 °K for carbon monoxide and hydrogen dimer and 2000–6000 °K for lithium hydride. As can be seen from the figures, the curves increase with enhances temperature for the diatomic molecules. Furthermore, we can see a good agreement between our results and experimental data. In Fig. 2a–d, we have presented Gibbs free energy for the diatomic molecules as a function of temperature at the same range in Fig. 1. We can see from the figures that the Gibbs free energy in Fig. 2b–d increases as the temperature increases for the selected diatomic molecules but in Fig. 2a, it decreases until 300 °K then it increases with enhancing temperature. Also, it is seen from the curves that there is fairly good agreement between our results and experimental values. Figure 3a–d displays the variation of enthalpy of IDEP with temperature for the selected diatomic molecules. Here, we have use the same range of temperature for the molecules. Like two previous comparisons, we can see a good agreement between our results and experimental data.

It is clear that the temperature variations of the specific heat at constant pressure for the diatomic molecules are slow. Accordingly, the range of variations of Gibbs free energy and enthalpy is higher than the specific heat. For example, the range of variations of the specific heat of N_2 is between 28 and 39 J/mol °K but its variations of enthalpy is between $-$ 6 and 205.4 J/mol. These results promise to very relevant to the study of thermochemical functions of different diatomic molecular systems [1, 7, 41–44]. Also this potential model has been used by other works [45, 46]. Furthermore, in Tables 3, 4 and 5, we have presented the deviations of our results and experimental data. These deviations maybe because of approximations that we have considered here.

5 Conclusion

In this work, we have solved the Schrödinger equation with the improved deformed exponential-type potential (IDEP) and have obtained the energy spectra of the model using the Greene-Aldrich approximation and a coordinate transformation. Applying the obtained energy spectra, we carry out a calculation of the vibrational partition function of the potential model for diatomic molecules under the lowest-order approximation. From the classical partition function obtained, we have derived explicit expressions for the thermodynamic functions, such as specific heat in constant pressure, Gibbs free energy and enthalpy. We have plotted the behaviors of the thermodynamic functions as functions of temperature T for N_2, CO, H_2 and LiH. The dependence of the thermodynamic functions on the temperature is discussed.

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