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Thermodynamic Properties for the Carbon Monoxide Molecule under the Influence of the Coulomb-Hulthen-Pöschl-Teller Potential

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ABSTRACT

In this study, we obtained the approximate *l*-states solutions of the Schrödinger equation interacting with a newly proposed potential known as the Coulomb-Hulthen-Pöschl-Teller (CHPT) by employing the parametric Nikiforov-Uvarov method. The analytical expressions for the energy eigenvalue as well as the vibrational mean energy, vibrational specific heat, vibrational free energy, and vibrational entropy for $X^1\Sigma^+$ states of carbon monoxide (CO) molecules have been presented in detail.

1. Introduction

In quantum mechanics, it is possible to describe the behavior of a physical system by a wavefunction that can be solved exactly for a given potential [1-5]. This is because the wavefunction provides all the necessary information about the quantum system. Knowing the exact solution to the Schrödinger equation plays a paramount role in quantum systems, but this exact solution is only possible for some potentials; thus approximation methods are usually adopted to arrive at the solution [6]. Some of the methods developed to find the approximate solution to the Schrödinger equation include; the asymptotic iteration method (AIM) [7-13], the super symmetric shape invariance method [14-19], the Nikiforov-Uvarov (NU) method [20-28], the variational method [29]. However, a good knowledge of these potentials helps in different fields of studies in physics such as atomic physics, condensed matter physics, high energy physics and particle physics [30-36]. The solutions obtained from the combination of two or more potentials give significant results having diverse application in quantum mechanics. In one of our recent publications [37], we obtained the approximate analytical solutions of the radial Schrödinger equation interacting with the Hellmann-generalized Morse potential, which is a combination of the Hellmann potential and the generalized Morse potential. Onate and Ojonuba [38] while combining the Coulomb potential, Yukawa potential and the inversely quadratic potential obtained the solutions of the radial Schrödinger equation. Their result could be applied to areas of physics such as plasma physics, solid state physics and atomic physics. The analytical solution of the Dirac equation with the Hellmann-Frost-Musulin potential, which is a combination of the Hellmann potential and the Frost-Musulin potential, was obtained by Onate et al. [39]. They also obtained the solution of the Klein Gordon equation with the combined potential (combination of the general Manning-Rosen potential, the hyperbolical potential and the Pöschl-Teller potential)

[40]. The Hellmann-Frost-Musulin potential can be applied to areas in condensed matter physics, atomic and molecular physics, whereas the combined potential finds application in areas like high energy physics, nuclear physics, atomic and molecular physics. Ita and Ikueba [41] solved the Schrödinger equation for the interaction of inversely quadratic Hellmann potential and the inversely quadratic potential for any angular momentum number, *l*. They obtained the energy eigenvalues and their corresponding eigenfunctions in terms of the Laguerre polynomials. Ikhdair and Sever [42] obtained the approximate solution of the Dirac equation with a combination of the reflectionless-type potential and the Rosen-Morse potential including the spin-orbit centrifugal term, using the Nikiforov-Uvarov method. In the same vein, Abdalla et al. [43] derived analytical solutions of the Schrödinger wave equation for some q-deformed potentials in terms of Huen functions. While Falaye et al. [44] in their paper, solved the one-dimensional Schrödinger equation with a combination of the Wood-Saxon potential, the Rosen-Morse potential and the symmetrical double well potential, using the Nikiforov-Uvarov method.

The stability of a system depends on the position of particles within the systems. A system with vibrating molecules/particles is usually unstable because the properties of the system such as entropy, internal energy, free energy and mean free energy change with respect to the particles' vibration. Hence, the study of thermodynamic properties becomes necessary. Dong et al. [45] studied the hidden symmetries and thermodynamic properties for harmonic oscillator plus an inverse square potential. Also, Dong and Cruz-Irisson [46] examined the energy spectrum and the thermodynamic properties for a modified Rosen-Morse potential. Baria and Jani [47] in 2012 studied some thermodynamic properties of liquid Na, K, Rb and Cs at various temperature measurements. Oyewunmi et al. [48] critically examined the thermodynamic properties and the approximate solutions of the Schrödinger equation with Shifted Deng-Fan potential model. Onate and Ojonubah [49] studied the thermodynamic properties of a system under the combination of the generalized Pöschl-Teller and hyperbolical potentials. In 2016, Onate and Onyeaju [50] investigated Dirac particles in the field of the Frost-Musulin diatomic potential and the thermodynamic properties.

In this paper, we propose a new potential model referred to as the Coulomb-Hulthen-Pöschl-Teller (CHPT) potential model which is lacking in literature. The CHPT potential model is a combination of the Coulomb potential, the Hulthen potential and the Pöschl-Teller potential. The combination of these potentials produces a potential well, which enables the molecules to be trapped thus aiding the calculation of the vibrational frequency of the molecules and also the thermodynamic properties of the vibrating system. Also, it is known that $CO\left(X^1\Sigma^+\right)$ molecule is photo dissociated by absorption of vacuum ultraviolet photons on discrete lines. For this reason, the thermodynamic properties of $X^1\Sigma^+$ states of CO will be investigated using the CHPT potential model. The CHPT potential model is given as:

$$V(r) = -\frac{A}{r} + \frac{Be^{-\eta r}}{1-e^{-\eta r}} - \frac{4Ce^{-2\alpha r}}{\left(1-e^{-2\alpha r}\right)^2}, \tag{1}$$

where A, B, C are potential strengths, α is the screening parameter and

$\eta = 2\alpha.$

We employ the approximation scheme in Eq. (2) suggested by Aldrich [51] and Wei and Dong [52] in order to obtain the *l* – states solution of the radial Schrödinger equation with potential (1) and to take care of the centrifugal term.

$$\frac{1}{r^2} \approx \frac{\eta^2}{(1-e^{-\eta r})^2}, \tag{2}$$

2. The parametric Nikiforov-Uvarov (NU) method

The Nikiforov-Uvarov (NU) method is based upon reducing the second-order linear differential equation to a hyper-geometric type equation [53]. By introducing an appropriate transformation $s = s(x)$, we can then write an equation of the form

$$\psi_n''(s) + \frac{\bar{\tau}(s)}{\sigma(s)}\psi_n'(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}\psi_n(s) = 0, \tag{3}$$

where $\sigma(s)$ and $\bar{\sigma}(s)$ are polynomials of degree two at most and $\bar{\tau}(s)$ is a polynomial of degree one at most. To use the parametric NU method, Tezcan and Sever [54-56] transformed Eq. (3) into the following form

$$\psi_n''(s) + \left(\frac{\lambda_1 - \lambda_2 s}{s(1-\lambda_3 s)}\right)\psi_n'(s) + \left(\frac{-\varsigma_1 s^2 + \varsigma_2 s - \varsigma}{s(1-\lambda_3 s)}\right)\psi_n(s) = 0. \tag{4}$$

From the parametric NU method, the bound state energy condition is obtained as [57, 58] (5)

$$n\lambda_2 - (2n+1)\lambda_5 + (2n+1)\left(\sqrt{\lambda_9} + \lambda_3\sqrt{\lambda_8}\right) + n(n-1)\lambda_3 + \lambda_7 + 2\lambda_3\lambda_8 + 2\sqrt{\lambda_8\lambda_9} = 0,$$

with the wave function as (6)

$$\psi_{n,l}(s) = N_{n,l}\, s^{\lambda_{12}} (1-\lambda_3 s)^{-\lambda_{12} - \frac{\lambda_{13}}{\lambda_3}} P_n^{\left(\lambda_{10}-1, \frac{\lambda_{11}}{\lambda_3} - \lambda_{10} - 1\right)}(1-2\lambda_3 s),$$

Where the parameters in Eq. (5) and Eq. (6) are given as follows (7)

$$\left.\begin{aligned} &\lambda_4 = \frac{1-\lambda_1}{2}, \lambda_5 = \frac{\lambda_2 - 2\lambda_3}{2}, \lambda_6 = \lambda_5^2 + \zeta_1, \lambda_7 = 2\lambda_4\lambda_5 - \zeta_2, \lambda_8 = \lambda_4^2 + \zeta_3, \\ &\lambda_9 = \lambda_3(\lambda_7 + \lambda_3\lambda_8) + \lambda_6, \lambda_{10} = \lambda_1 + 2\lambda_4 - 2\sqrt{\lambda_8}, \lambda_{11} = \lambda_2 - 2\lambda_5 + 2\left(\sqrt{\lambda_9} - \lambda_3\sqrt{\lambda_8}\right), \\ &\lambda_{12} = \lambda_4 - \sqrt{\lambda_8}, \lambda_{13} = \lambda_5 - \left(\sqrt{\lambda_9} - \lambda_3\sqrt{\lambda_8}\right) \end{aligned}\right\}.$$

3. Radial solution to the Schrödinger equation

The radial Schrödinger equation is of the form [38].

$$\frac{d^2R(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2}\left\{E - V(r) - \frac{L\hbar^2}{2\mu r^2}\right\}\right]R(r) = 0, \tag{8}$$

where $L = l(l+1)$, μ is the particle mass, E is the non-relativistic energy and $V(r)$ is the interacting potential. If we substitute our proposed potential model in Eq. (1) and the approximation scheme in Eq. (2) into the Schrödinger equation (8), we obtain

$$\left[\frac{d^2}{dr^2}+\frac{2\mu E}{\hbar^2}-\frac{2\mu}{\hbar^2}\left\{-\frac{A}{r}+\frac{Be^{-2\alpha r}}{1-e^{-2\alpha r}}-\frac{4Ce^{-2\alpha r}}{\left(1-e^{-2\alpha r}\right)^2}\right\}-\frac{L}{r^2}\right]R(r). \tag{9}$$

In applying the NU method, a transformation variable of the form $s=e^{-2\alpha r}$ is defined and substituted into Eq. (9) to get

$$\left[\frac{d^2}{ds^2}+\frac{(1-s)}{s(1-s)}\frac{d}{ds}+\frac{1}{s^2(1-s^2)}\left\{-\kappa_1 s^2+\kappa_2 s-\kappa_3\right\}\right]R(s)=0, \tag{10}$$

where (11)

$$\kappa_1=-\frac{\mu(E+B)}{2\alpha^2\hbar^2},\kappa_2=-\frac{\mu}{2\alpha^2\hbar^2}(2E+2A\alpha+B-4C),\kappa_3=-\frac{\mu}{2\alpha^2\hbar^2}\left(E+2A\alpha-\frac{2\alpha^2\hbar^2L}{\mu}\right).$$

From the comparison of Eq. (4) and Eq. (10), we obtain the following parametric constants

$$\lambda_1=\lambda_2=\lambda_3=1,\lambda_4=0,\lambda_5=-\frac{1}{2},\lambda_6=\frac{1}{4}+\kappa_1,\lambda_7=-\kappa_2,\lambda_8=\kappa_3,$$

$$\lambda_9=-\kappa_2+\kappa_3+\kappa_1+\frac{1}{4},\lambda_{10}=1+2\sqrt{\kappa_3},\lambda_{11}=2\left(1+\sqrt{\kappa_3}+\sqrt{\lambda_9}\right), \tag{12}$$

$$\lambda_{12}=\sqrt{\kappa_3},\lambda_{13}=-\frac{1}{2}-\sqrt{\lambda_9}+\sqrt{\kappa_3}.$$

Substituting the appropriate parametric constants obtained in Eq. (12) into Eq. (5), we obtain the energy equation of our proposed Coulomb-Hulthen-Pöschl-Teller potential as:

$$E_{n,l}=\frac{2\alpha^2\hbar^2}{\mu}\left\{L-\frac{A\mu}{\alpha\hbar^2}-\left[\frac{\frac{2\mu}{\alpha^2\hbar^2}\left(C+\frac{\alpha A}{2}-\frac{B}{4}-\frac{\alpha^2\hbar^2(2l+1)^2}{4\mu}-\frac{\alpha^2\hbar^2n(n+1)}{2\mu}\right)-\left(n+\frac{1}{2}\right)\sqrt{(2l+1)^2-\frac{8\mu C}{\alpha^2\hbar^2}}}{1+2n+\sqrt{(2l+1)^2-\frac{8\mu C}{\alpha^2\hbar^2}}}\right]^2\right\}. \tag{13}$$

4. The thermodynamic properties of the Coulomb-Hulthen-Pöschl-Teller potential (CHPT)

In this section, we study the thermodynamic properties of CO, a diatomic molecule with the CHPT potential model; the energy of the system E_n is obtained as

$$E_n=\frac{2\alpha^2\hbar^2}{\mu}\left[\Lambda_1-\left(\frac{\Lambda_2}{2(n+\tau)}+\frac{n+\tau}{2}\right)^2\right], \tag{14}$$

$$n=0,1,2,.....<n_{\max}=[\varpi],$$

where (15)

$$\Lambda_1=-\frac{2A\mu}{\alpha\hbar^2},\ \Lambda_2=\frac{\mu}{\alpha^2\hbar^2}\left(A\alpha-\frac{B}{2}+6C-\frac{3\alpha^2\hbar^2}{8\mu}-\frac{\alpha^2\hbar^2}{4\mu}\right),$$

$$\tau=\frac{1}{2}\left[1+\sqrt{1-\frac{8\mu C}{\alpha^2\hbar^2}}\right].$$

We have introduced in Eq. (14) $[\varpi]$ to represent the largest inferior given by $\varpi = -\tau + \sqrt{\Lambda_1} \pm \sqrt{\Lambda_1 - \Lambda_2}$ for mathematical simplicity.

The vibrational partition function for the CO molecule is obtained as

$$Z(\beta,\varpi) = \sum_{n=0}^{\varpi} e^{-\beta E_n},\ \beta = \frac{1}{\mathrm{kT}}, \tag{16}$$

where k is the Boltzmann constant. On substituting Eq. (13) into Eq. (16) yields (17)

$$Z(\beta,\varpi) = \sum_{n=0}^{\varpi} e^{\frac{\beta\alpha^2\hbar^2}{\mu}(\Lambda_2 - 2\Lambda_1) + \frac{\beta\alpha^2\hbar^2\Lambda_2^2}{2\mu(n+\tau)^2} + \frac{\beta\alpha^2\hbar^2}{2\mu}(n+\tau)^2}.$$

In the classical limit, the summation in Eq. (17) can be replaced by an integral (18)

$$Z(\beta,\varpi) = \int_0^{\varpi} e^{\frac{\beta\alpha^2\hbar^2}{\mu}(\Lambda_2 - 2\Lambda_1) + \frac{\beta\alpha^2\hbar^2\Lambda_2^2}{2\mu\rho^2} + \frac{\beta\alpha^2\hbar^2}{2\mu}\rho^2} d\rho,\ \ \rho=(n+\tau).$$

$$Z(\beta,\varpi) = \frac{1}{2} e^{\beta\Lambda_3}\sqrt{\Lambda_4\beta}\left\{\frac{2\varpi e^{\frac{\Lambda_4\beta}{\varpi^2}}}{\sqrt{\Lambda_4\beta}} - \frac{2\sqrt{\Lambda_4\beta}\sqrt{\pi}\,\mathrm{Erfi}\left(\frac{\sqrt{\Lambda_4\beta}}{\varpi}\right)}{\sqrt{\Lambda_4\beta}} - 2\sqrt{\pi}\right\}, \tag{19}$$

where (20)

$$\Lambda_3 = \frac{\alpha^2\hbar^2}{2\mu}\left[1 + 2\left(\Lambda_2 - 2\Lambda_1\right)\right],\ \Lambda_4 = \frac{\alpha^2\hbar^2\Lambda_2^2}{2\mu}.$$

From the vibrational partition function of Eq. (19), the thermodynamic properties of molecular CO can now be determined as follows:

4.1: The vibrational energy U:

$$U(\beta) = -\frac{\partial}{\partial\beta}\ln Z_{vib}(\beta) \tag{21}$$

$$= e^{-\beta\Lambda_3\rho^2}\Lambda_5\left\{2\left(\frac{\Lambda_3\rho^2}{2}e^{\beta\Lambda_3\rho^2}\sqrt{\beta\Lambda_2}(\Lambda_5) + \frac{e^{\beta\Lambda_3\rho^2}(\Lambda_5)\Lambda_2}{\sqrt{\beta\Lambda_2}} - \frac{e^{\beta\Lambda_3\rho^2}}{2}\varpi e^{\frac{\beta\Lambda_2}{\varpi^2}}\right)\right\},$$

where (22)

$$\Lambda_5 = \frac{2\varpi e^{\frac{\beta\Lambda_2}{\varpi^2}}}{\sqrt{\beta\Lambda_2}} - 2\sqrt{\pi}\,\mathrm{Erfi}\left(\frac{\sqrt{\beta\Lambda_2}}{\varpi}\right) - 2\sqrt{\pi}\ .$$

4.2: Vibrational specific heat capacity C:

$$C(\beta) = \frac{\partial}{\partial T}U = -k\beta^2\frac{\partial}{\partial\beta}U = k\beta^2\left\{\frac{1}{e^{\beta\Lambda_3\rho^2}\sqrt{\beta\Lambda_2}(\Lambda_5)}\left[2\left(\Delta_6 - \frac{\Lambda_7}{8} - \Lambda_8\left(\Lambda_3\rho^2\right)\right)\right]\right. \tag{23}$$

$$\left. - \frac{1}{e^{\beta\Lambda_3\rho^2}\left(\beta\Lambda_2\right)^{3/2}(\Lambda_5)}\left(\Lambda_8\Lambda_2\right) + \frac{1}{e^{\beta\Lambda_3\rho^2}\left(\beta^2\Lambda_2\right)(\Lambda_5)^2}2\left(\Lambda_8\Lambda_2\right)\varpi e^{\frac{\beta\Lambda_2}{\varpi^2}}\right\},$$

where (24)

$$\Lambda_6 = \left(\frac{\Lambda_3\rho^2}{2}\right)^2 e^{\beta\Lambda_3\rho^2}\sqrt{\beta\Lambda_2}(\Lambda_5) + \frac{\Lambda_3\rho^2 e^{\beta\Lambda_3\rho^2}(\Lambda_5)\Lambda_2}{2\sqrt{\beta\Lambda_2}} - \frac{\Lambda_3\rho^2 e^{\beta\Lambda_3\rho^2}\varpi e^{\frac{\beta\Lambda_2}{\varpi^2}}}{\beta},$$

$$\Lambda_7 = \frac{e^{\beta\Lambda_3\rho^2}(\Lambda_5)\Lambda_2^2}{(\beta\Lambda_2)^{3/2}} + \frac{e^{\beta\Lambda_3\rho^2}\varpi e^{\frac{\beta\Lambda_3}{\varpi^2}}}{4\beta^2} - \frac{e^{\beta\Lambda_3\rho^2}\Lambda_2 e^{\frac{\beta\Lambda_3}{\varpi^2}}}{\beta\varpi},$$

$$\Lambda_8 = \frac{\Lambda_3\rho^2}{2}e^{\beta\Lambda_3\rho^2}\sqrt{\beta\Lambda_2}(\Lambda_5) + \frac{\Lambda_3\rho^2 e^{\beta\Lambda_3\rho^2}(\Lambda_5)\Lambda_2}{4\sqrt{\beta\Lambda_2}} - \frac{e^{\beta\Lambda_3\rho^2}\varpi e^{\frac{\beta\Lambda_2}{\varpi^2}}}{2\beta},$$

4.3: Vibrational mean free energy F:

$$F(\beta) = -kT\ln Z_{vib}(\beta) = -\frac{1}{\beta}\ln\left[\frac{1}{2}e^{\beta\Lambda_3}\sqrt{\Lambda_4\beta}\left\{\frac{2\varpi e^{\frac{\Lambda_4\beta}{\varpi^2}}}{\sqrt{\Lambda_4\beta}} - \frac{2\sqrt{\Lambda_4\beta}\sqrt{\pi}\,\mathrm{Erfi}\left(\frac{\sqrt{\Lambda_4\beta}}{\varpi}\right)}{\sqrt{\Lambda_4\beta}} - 2\sqrt{\pi}\right\}\right]. \quad (25)$$

4.4: Vibrational entropy S:

$$S(\beta) = k\ln Z_{vib}(\beta) + kT\frac{\partial}{\partial T}\ln Z_{vib}(\beta) = \quad (26)$$

$$k\ln\left[\frac{1}{2}e^{\beta\Lambda_3}\sqrt{\Lambda_4\beta}\left\{\frac{2\varpi e^{\frac{\Lambda_4\beta}{\varpi^2}}}{\sqrt{\Lambda_4\beta}} - \frac{2\sqrt{\Lambda_4\beta}\sqrt{\pi}\,\mathrm{Erfi}\left(\frac{\sqrt{\Lambda_4\beta}}{\varpi}\right)}{\sqrt{\Lambda_4\beta}} - 2\sqrt{\pi}\right\} + \mathrm{kT}\Lambda_1\right].$$

5. Some Theoretic quantities and the Coulomb-Hulthen-Pöschl-Teller potential (CHPT)

In this section, we calculate the Information energy, Tsallis entropy and Rényi entropy using the probability density obtained from the normalized radial wave function. To begin, we first calculate the normalized wave function. Given the radial wave function as:

$$\left[R_{n\ell}(y)\right]^2 = N_{n\ell}^2 y^{2a}(1-y)^{2b}\left[P_n^{(2a,b)}(1-2y)\right]^2.\ y = e^{-2\alpha}. \quad (27)$$

which is equal to the probability density $\rho(y)$, we can easily calculate the theoretic quantities mentioned above. Where $a = \sqrt{-\frac{\mu(E_{n\ell}+\alpha A)}{2\alpha^2\hbar^2} + \ell(\ell+1)}$ and $b = \sqrt{(1+2\ell)^2 - \frac{8\mu C}{\alpha^2\hbar^2}}$. Normalizing the radial wave function, we have

$$\int_1^0 \left[R_{n\ell}(y)\right]^2 dy = 1,\ y = e^{-2\alpha}. \quad (28)$$

Substitute the value of $R_{n\ell}(y)$, we have (29)

$$\frac{N_{n\ell}^2}{4\alpha}\int_{-1}^{1}(1-s)^{u-1}(1+s)^{\frac{1+v}{2}}\left[P_n^{(u,v)}(s)\right]^2 ds=1,$$

where we have used: $2a=u,\ b=v,\ x=1-2y$ and $\frac{1+x}{2}=1-\left(\frac{1-s}{2}\right)$. Using integral of the form

$$\int_{-1}^{1}(1-x)^{t-1}(1+x)^{k}\left[P_n^{(t,k)}(x)\right]^2 dx=\frac{2^{t+k}\Gamma(t+n+1)\Gamma(k+n+1)}{n!t\Gamma(t+k+n+1)}, \tag{30}$$

we have the normalization constant as:

$$N_{n\ell}=2\sqrt{\frac{\alpha n!u\,\Gamma\left(\frac{2u+v+3+2n}{2}\right)}{2^{\frac{2U+v+1}{2}}\Gamma(u+n+1)\Gamma\left(\frac{v+3+2n}{2}\right)}}. \tag{31}$$

5.1: Information energy

Information energy is defined as

$$E(\rho)=4\pi\int_{0}^{\infty}\rho(r)dr. \tag{32}$$

$$E(\rho)=4\pi\int_{1}^{0}\rho(y)dy.\ y=\exp(-2\alpha r). \tag{33}$$

$$E(\rho)=4\pi\int_{-1}^{1}\rho(z)dz.\ z=1-2y. \tag{34}$$

Substitute the value of the probability density, we have

$$E(\rho)=4\pi N_{n\ell}^2\int_{-1}^{1}\left(\frac{1-z}{2}\right)^{u-1}\left(\frac{1+z}{2}\right)^{\frac{1+v}{2}}\left[P_n^{(u,v)}(z)\right]^2 dz. \tag{35}$$

Using integral of the form

$$\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{c}\left(\frac{1+y}{2}\right)^{d}\left[P_n^{(u,v)}(y)\right]^2 dy=\frac{2\Gamma(c+n+1)\Gamma(d+n+1)}{n!\Gamma(c+d+2n+1)\Gamma(c+d+n+1)}, \tag{36}$$

and the normalization constant calculated above, the information energy is obtain as

$$E(\rho)=\frac{100.544\alpha u\Gamma(u+n)}{2^{\frac{1+v+2u}{2}}\Gamma(u+n+1)\Gamma\left(\frac{2u+4n+v+3}{2}\right)}. \tag{37}$$

$$E(\rho)=\frac{221.68u\Gamma(u+n)}{2^{\frac{1+v+2u}{2}}\Gamma(u+n+1)\Gamma\left(\frac{2u+4n+v+3}{2}\right)}. \tag{38}$$

5.2: Tsallis entropy

The Tsallis entropy is defined as:

$$T(q)=\frac{1}{q-1}\left(1-4\pi\int_0^{\infty}\rho(r)^q dr\right).\ q\neq 1 \tag{39}$$

Substituting for the probability density, we have (40)

$$T(q)=\frac{1}{q-1}\left[1-4\pi\int_{-1}^{1}\left(N_{n\ell}^2\left(\frac{1-z}{2}\right)^{u-1}\left(\frac{1+z}{2}\right)^{\frac{1+v}{2}}\left[P_n^{(u,v)}(z)\right]^2\right)^q dz\right],$$

Using integral of the form in Eq. (36), the Tsallis entropy is obtain as (41)

$$T(q)=\frac{1}{q-1}-\frac{12.568}{q-1}\left(\frac{4\alpha u\Gamma(u+n)}{2^{\frac{1+v+2u}{2}}\Gamma(u+n+1)\Gamma\left(\frac{2u+4n+v+3}{2}\right)}\right)^q.$$

$$T(q)=\frac{1}{q-1}-\frac{12.568}{q-1}\left(\frac{8.8192u\Gamma(u+n)}{2^{\frac{1+v+2u}{2}}\Gamma(u+n+1)\Gamma\left(\frac{2u+4n+v+3}{2}\right)}\right)^q. \tag{42}$$

5.3: Rényi entropy

The Rényi entropy is defined as

$$R(q)=\frac{1}{1-q}\log 4\pi\int_0^{\infty}\rho(r)^q dr.\ q\neq 1 \tag{43}$$

Substituting for the probability density, we have (44)

$$R(q)=\frac{1}{q-1}\log 4\pi\int_{-1}^{1}\left(N_{n\ell}^2\left(\frac{1-z}{2}\right)^{u-1}\left(\frac{1+z}{2}\right)^{\frac{1+v}{2}}\left[P_n^{(u,v)}(z)\right]^2\right)^q dz,$$

Substituting for the normalization constant with the integral in Eq. (36), the Rényi entropy is obtain as (45)

$$R(q)=\frac{1.0993}{1-q}\left(\frac{2^{\frac{5-2u-v}{2}}\alpha u\Gamma(u+n)}{\Gamma(u+n+1)\Gamma\left(\frac{2u+4n+v+3}{2}\right)}\right)^q.$$

$$R(q)=\frac{1.0993}{1-q}\left(\frac{17.6384\times 2^{-\left(\frac{1+2u+v}{2}\right)}\alpha u\Gamma(u+n)}{\Gamma(u+n+1)\Gamma\left(\frac{2u+4n+v+3}{2}\right)}\right)^q. \tag{46}$$

6. Discussion of Results

Special cases:

When $A=0,$ the energy Equation (13) becomes

$$E_{n,l}=\frac{2\alpha^2\hbar^2}{\mu}\left\{L-\left[\frac{\frac{2\mu}{\alpha^2\hbar^2}\left(C-\frac{B}{4}-\frac{\alpha^2\hbar^2(2l+1)^2}{4\mu}-\frac{\alpha^2\hbar^2n(n+1)}{2\mu}\right)-\left(n+\frac{1}{2}\right)\sqrt{(2l+1)^2-\frac{8\mu C}{\alpha^2\hbar^2}}}{1+2n+\sqrt{(2l+1)^2-\frac{8\mu C}{\alpha^2\hbar^2}}}\right]^2\right\}. \quad (47)$$

If $B=0$, the energy equation becomes (48)

$$E_{n,l}=\frac{2\alpha^2\hbar^2}{\mu}\left\{L-\frac{A\mu}{\alpha\hbar^2}-\left[\frac{\frac{2\mu}{\alpha^2\hbar^2}\left(C+\frac{\alpha A}{2}-\frac{\alpha^2\hbar^2(2l+1)^2}{4\mu}-\frac{\alpha^2\hbar^2n(n+1)}{2\mu}\right)-\left(n+\frac{1}{2}\right)\sqrt{(2l+1)^2-\frac{8\mu C}{\alpha^2\hbar^2}}}{1+2n+\sqrt{(2l+1)^2-\frac{8\mu C}{\alpha^2\hbar^2}}}\right]^2\right\}.$$

If $C=0$, the energy equation turns to (49)

$$E_{n,l}=\frac{2\alpha^2\hbar^2}{\mu}\left\{L-\frac{A\mu}{\alpha\hbar^2}-\left[\frac{\frac{2\mu}{\alpha^2\hbar^2}\left(\frac{\alpha A}{2}-\frac{B}{4}-\frac{\alpha^2\hbar^2(2l+1)^2}{4\mu}-\frac{\alpha^2\hbar^2n(n+1)}{2\mu}\right)-(2l+1)\left(n+\frac{1}{2}\right)}{2(n+l+1)}\right]^2\right\}.$$

The vibrational partition function for the CHPT molecular potential model has been obtained at the classical limit. The experimental data for $CO\left(X^1\Sigma^+\right)$ molecule was taken from the spectroscopic experimental data reported [59]. Accordingly, we have adopted the following values $A=1.128$Å, $B=0.149936$, $\alpha=2.2048$Å^{-1}, $\mu=1.146x10^{-23}g$ and $C=90531\,cm^{-1}$ for the potential parameters used in this present study. In Figure 1, the partition function increases monotonically with an increase in β at a high temperature range. Also, the molecule starts dissociating at energy of about 5J. This can be seen in Figure 2 with the internal energy decreasing monotonically with an increase in β. The specific heat capacity of the molecule dissociated at various values of β except at the value near zero as shown in Figure 3. This shows that at low temperature range, the spread of $CO\left(X^1\Sigma^+\right)$ is reduced. The vibrational free energy of the system also shows some sensitivity to the range of temperature with a negative value (Figure 4) while Figure 5 shows that the entropy of the molecule increases linearly with an increase in β. In Table 1, we presented the numerical values for the Coulomb-Hulthén Pöschl-Teller potential. The energy eigenvalue decreases as the quantum number increases.

7. Conclusion

We haveinvestigated the thermodynamic properties of the carbon monoxide molecule $CO\left(X^1\Sigma^+\right)$ using the CHPT potential model. The eigenvalue obtained from the newly proposed potential model, is then applied to obtain the partition function. The explicit expressions for the thermodynamic properties, such as: vibrational mean energy U, specific heat C, free energy F, and entropy S of the system. The effect of the temperature parameter β on the various thermodynamics quantities for the $X^1\Sigma^+$ states of CO have been investigated in detail. The theoretic quantities such as information energy, Rényi entropy and Tsallis entropy are calculated.

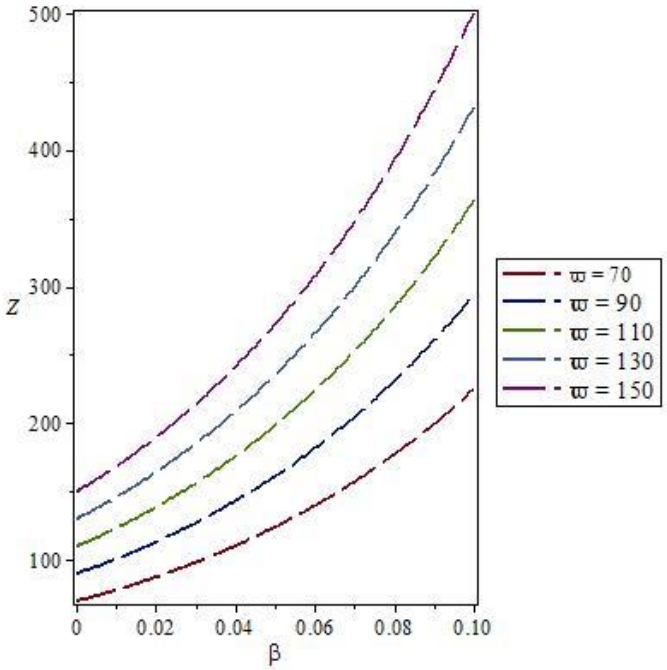

Figure 1: Vibrational partition function for different values of ϖ, as β increased monotonically with Z

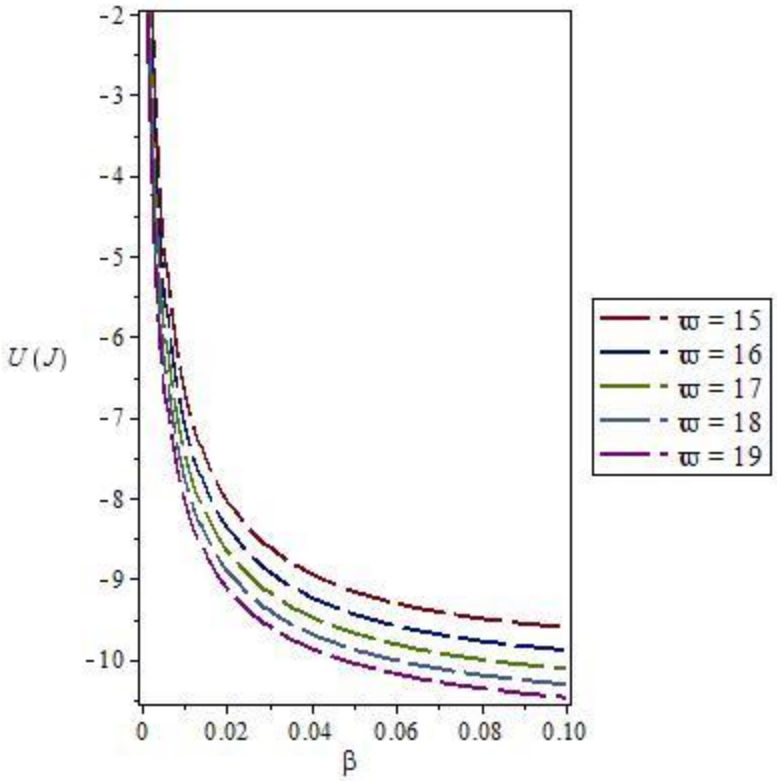

Figure 2: Variation of internal energy U with β

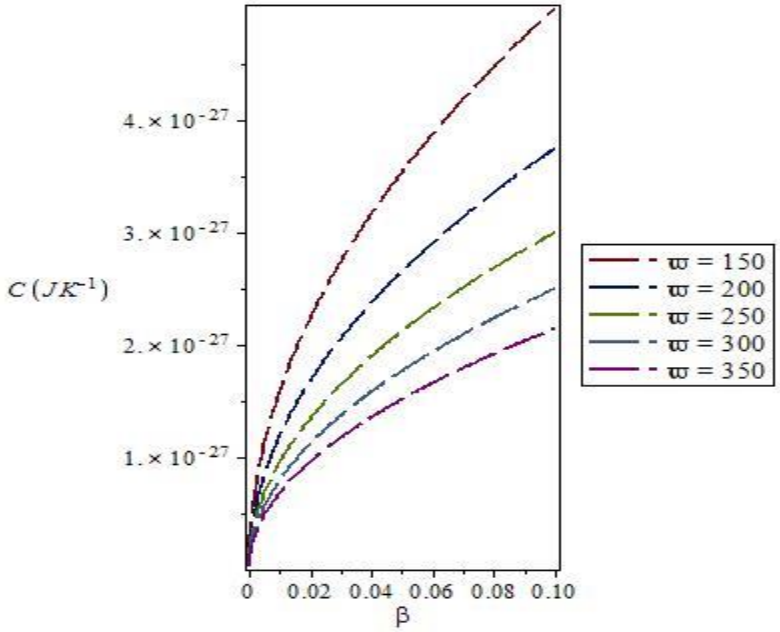

Figure 3: Variation of the specific heat capacity with β

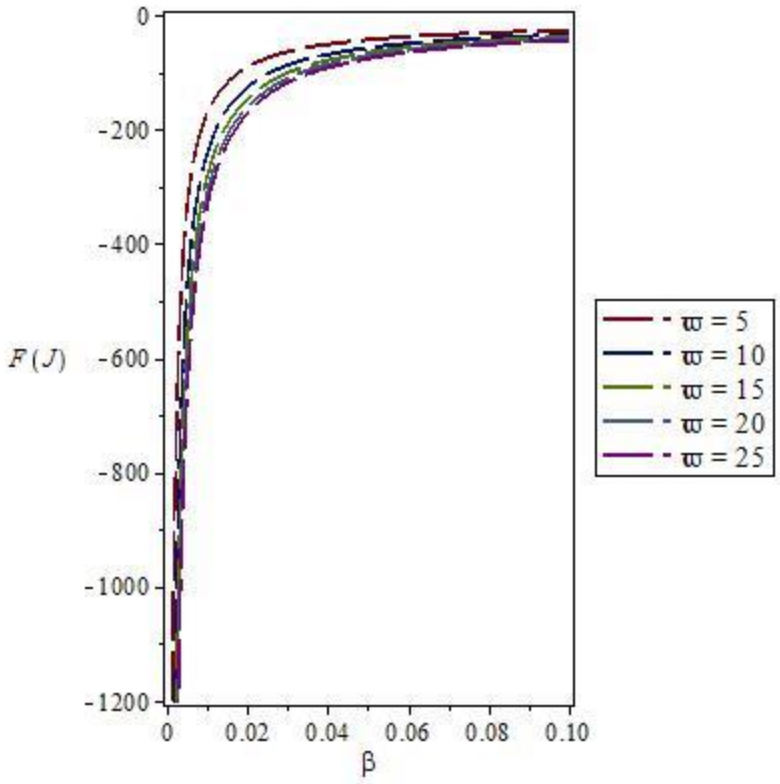

Figure 4: Variation of the vibrational mean free energy with β

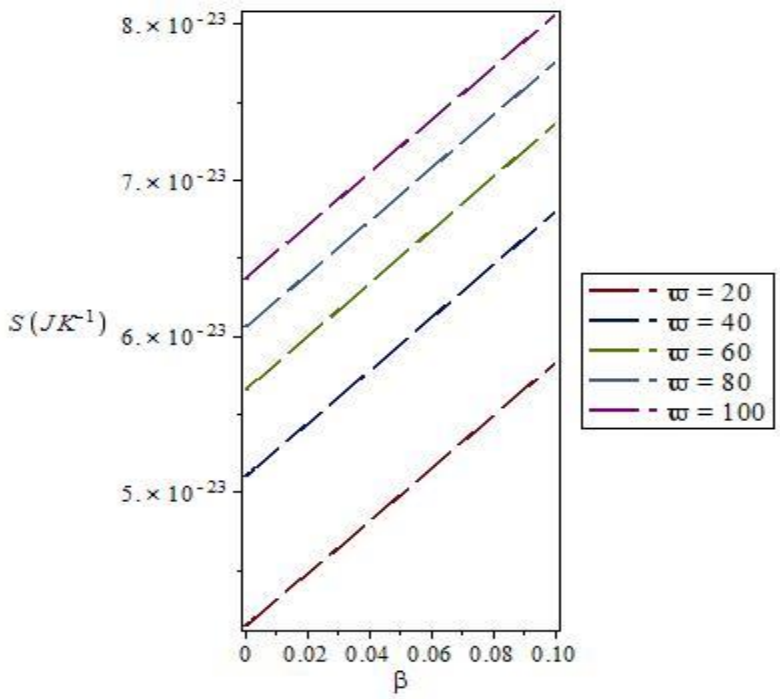

Figure 5: Variation of the vibrational entropy with β

Table 1: Energy spectra for Coulomb-Hulthén Pöschl-Teller potential for *2p*, *3p* and *3d* for three values of α.

state	α	$B=A=-C=1$	$B=2A=-2C=2$	$2B=A=-2C=2$
2p	0.05	-1.606059113	-2.270353834	-1.646249575
	0.10	-1.598731728	-2.232544041	-1.685811919
	0.15	-1.546183422	-2.143605317	-1.688422695
	0.20	-1.454652035	-2.011157803	-1.661349015
3p	0.05	-1.676400130	-2.329861950	-1.717237391
	0.10	-1.747851812	-2.365182631	-1.836523320
	0.15	-1.782073253	-2.362655259	-1.925654008
	0.20	-1.783770598	-2.328070513	-1.989020959
3d	0.05	-1.554926971	-2.211234137	-1.595883913
	0.10	-1.404290670	-2.008428375	-1.497046307
	0.15	-1.136625999	-1.673084350	-1.296295388
	0.20	-0.781328125	-1.240312500	-1.025078125

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9. Conflict of Interest

There is no conflict of interest associated with this work.

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