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# Applications of Hellmann-Feynman Theorem (HFT) to Angle Dependent Yukawa Potential of Diatomic Molecules

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**Abstract**

We have applied Hellmann-Feynman Theorem (HFT) to the bound state solutions of angle dependent Yukawa potential model for five selected diatomic molecules. The diatomic molecules we have investigated are $H_2, CO, NO, N_2$ and $Ar_2$. Also we used the obtained potential parameters and energy eigenvalues of these selected diatomic molecules to compute the expectation values of $\langle r^{-2} \rangle$ and $\langle r^{-1} \rangle$ for the radial part of the system. The expectation values for the kinetic energy $\langle T \rangle$ and the squared momentum $\langle p^2 \rangle$ are also studied numerically for both the radial and the effective potential of the system.

**Keywords:** Expectation values, Hellmann-Feynmann theorem, diatomic molecules, Yukawa potential, angle dependent potential.

## 1.0 Introduction

Hellmann-Feynman theorem (HFT) is commonly used in the calculation of intermolecular forces in molecules. However, in order to engage HFT in calculating the expectation values, one then need to promote the fixed parameters which appears in the Hamiltonian to be continuous variable in order to ease the mathematical purpose of taking the derivatives. This theorem assures that a non-degenerate eigenvalue of hermitian operator in a parameter dependent eigen system varies with respect to the parameter according to the formula [1]:

$$\frac{\partial E_n(q)}{\partial q} = \left\langle \Psi(q) \right| \frac{\partial H(q)}{\partial q} \left| \Psi(q) \right\rangle, \qquad 1$$

provided that the associated normalized eigenfunction $\psi(q)$ is continous with respect to the parameter $q$. This equation is a useful tool which have been used in many areas of physics and specially in solid state and nuclear physics, atomic and molecular physics, with the pioneering work of Feynman[2] moving the, so called, electrostatic theorem[3].

Noncentral potential has been studied in various fields of nuclear physics and quantum chemistry which could be used for the interaction between deformed pair of nuclei and ring shaped molecules like benzenes [4-8]. Yukawa potential is one of the short ranged potentials that have been studied in physics, they have Coulombic behavior for small $r$ and are exponentially damped for large $r$, and they have limited number of bound states characterized by the presence of the screening parameter $\alpha$ [9-13]. This model receives great attention due to the fact that it plays an important role in high energy and particle physics, atomic physics, chemical physics, gravitational plasma physics and solid state physics. In solid state physics and atomic physics, it is called the Thomas-Fermi or screened Coulomb potential while in plasma physics it is known as the Debye-Huckel potential [14,15].

Therefore the motivation of this present work is to extend the work of one of us in ref. [16] by evaluating the expectation values of Yukawa plus angle dependent system reported as

$$V(r,\theta) = -\frac{V_0 e^{-\alpha r}}{r} + \frac{\hbar^2}{2\mu}\left(\frac{\gamma + \beta\cos^2\theta + \eta\cos^4\theta}{r^2\cos^2\theta\sin^2\theta}\right). \qquad 2$$

Our potential was suggested based on the motivation derived from the applications of Yukawa potential and ring-shaped potential. The former as already mentioned in the paper has a lot of applications in physics such as in atomic physics, chemical physics, plasma physics etc. The ring-shaped potential is to study the interaction between deformed pair of nuclei and ring-shaped molecules like benzene.

In this paper, we have applied Hellmann-Feynman theorem (HFT) to the already obtained bound state solutions of Yukawa plus ring-shaped potential model presented in ref. [16] for the five selected diatomic molecules such as $H_2, CO, NO, N_2$ and $Ar_2$.

The solutions the potential in Eq.(2) were obtained using the parametric generalization of the Nikiforov-Uvarov(NU) method [17, 18]

$$\psi''(s)+\frac{(c_1-c_2s)}{s(1-c_3s)}\psi'(s)+\frac{1}{s^2(1-c_3s)^2}\left[-\xi_1s^2+\xi_2s-\xi_3\right]\psi(s)=0. \qquad 3$$

This methods generate the following energy and wave function equations respectively as follows

$$c_2n-(2n+1)c_5+(2n+1)\left(\sqrt{c_9}+c_3\sqrt{c_8}\right)+n(n-1)c_3+c_7+2c_3c_8+2\sqrt{c_8c_9}=0, \qquad 4$$

$$\psi(s)=N_{nl}s^{c_{12}}\left(1-c_3s\right)^{-c_{12}-\frac{c_{13}}{c_3}}P_n^{\left(c_{10}-1,\frac{c_{11}}{c_3}-c_{10}-1\right)}\left(1-2c_3s\right), \qquad 5$$

where

$$\begin{aligned}&c_4=\frac{1}{2}(1-c_1),\ c_5=\frac{1}{2}(c_2-2c_3),\ c_6=c_5^2+\xi_1,\ c_7=2c_4c_5-\xi_2,\ c_8=c_4^2+\xi_3,\\&c_9=c_3c_7+c_3^2c_8+c_6,\ c_{10}=c_1+2c_4+2\sqrt{c_8},\ c_{11}=c_2-2c_5+2\left(\sqrt{c_9}+c_3\sqrt{c_8}\right),\\&c_{12}=c_4+\sqrt{c_8},\ c_{13}=c_5-\left(\sqrt{c_9}+c_3\sqrt{c_8}\right)\end{aligned} \qquad 6$$

and $P_n^{(\alpha,\beta)}(s)$ is the orthogonal Jacobi polynomial. For details on NU method the readers can see ref. [16,17,18].

## 2.0 Review of solutions of Yukawa plus ring-shaped potential

By Tailor expanding Eq.(2) and marking use of the first two terms, the radial energy for the system was obtained as[16]

$$E_{nl}=V_0\alpha-\frac{2\mu}{\hbar^2}\frac{V_0^2}{\left[(2n+1)+2\sqrt{\lambda+\frac{1}{4}}\right]^2}. \qquad 7$$

and the corresponding radial wave function For this system was obtained as:

$$R(r)=N_nr^{-\frac{1}{2}+v}e^{-\sqrt{\varepsilon+B'}r}L_n^{2v}\left(2\sqrt{\varepsilon+B'}r\right) \qquad 8$$

where $v=\sqrt{\lambda+\frac{1}{4}}$ and $N_n$ is a normalization constant.

Furthermore angular wave function for the system was obtained as

$$\Theta(s)=N_ms^{\frac{1}{4}+\frac{1}{2}\sqrt{\gamma+\frac{1}{4}}}\left(1-s\right)^{\frac{1}{2}\sqrt{m^2+\gamma+\beta+\eta}}\times P_n^{\left(\sqrt{\gamma+\frac{1}{4}},\sqrt{m^2+\gamma+\beta+\eta}\right)}(1-2s) \qquad 9$$

Equation (9) can further be written as

$$\Theta(\theta)=N_m(\cos\theta)^{\frac{1}{2}+\sqrt{\gamma+\frac{1}{4}}}(\sin\theta)^{\sqrt{m^2+\gamma+\beta+\eta}}\times P_n^{\left(\sqrt{\gamma+\frac{1}{4}},\sqrt{m^2+\gamma+\beta+\eta}\right)}(-\cos2\theta), \qquad 10$$

where $N_m$ is a normalization constant.

After simple manipulations, effective energy or the total energy of the Yukawa plus angle dependent potential yielded the following energy spectra [16]:

$$E_{nlm}=V_0\alpha-\frac{2\mu}{\hbar^2}\frac{V_0^2}{\left[(2n+1)+2\delta\right]^2} \qquad 11$$

where $\delta=\sqrt{\begin{aligned}&4\left(n+\frac{1}{2}\right)^2+2(2n+1)\left(\sqrt{m^2+\gamma+\beta+\eta}+\sqrt{\gamma+\frac{1}{4}}\right)\\&+2\sqrt{\left(m^2+\gamma+\beta+\eta\right)\left(\gamma+\frac{1}{4}\right)}+m^2+2\gamma+\beta+\frac{1}{4}\end{aligned}}$

with the corresponding effective or total wave function as

$$\psi(r,\theta,\varphi)=\frac{N_{nm}}{\sqrt{2\pi}}r^{-\frac{1}{2}+v}e^{im\varphi-\sqrt{\varepsilon+B'}r}L_n^{2v}\left(2\sqrt{\varepsilon+B'}r\right) \times(\cos\theta)^{\frac{1}{2}+\sqrt{\gamma+\frac{1}{4}}}(\sin\theta)^{\sqrt{m^2+\gamma+\beta+\eta}} \times P_n^{\left(\sqrt{\gamma+\frac{1}{4}},\sqrt{m^2+\gamma+\beta+\eta}\right)}(-\cos 2\theta) \qquad 12$$

where $N_{nm}$ is the normalization constant.

Diatomic molecular potential are very important to describe the intramolecular and intermolecular interactions and atomic pair correlations in quantum mechanics [19, 20]. We shall apply the exact solution of Schrödinger equation for some selected diatomic molecules for the s-wave by setting $V_0 = D_e r_e$ in Eq.(11).

$$E_{nlm} = D_e r_e \alpha - \frac{2\mu}{\hbar^2}\frac{(D_e r_e)^2}{[(2n+1)+2\delta]^2} \qquad 13$$

Where $D_e$ is the dissociation energy (interaction energy between two atoms in a molecular system). And $r_e$ is the distance of separation between the atoms. Setting $\gamma=\beta=\eta=1$ and making use of table 1 we obtain numerical values for our total energy eigenvalue. The values for $\gamma=\beta=\eta=1$ is used arbitrarily for uniformity. However, depending on the purpose and interest one may use any different value for these potential parameters. The potential is a short range potential and the range of values for $\alpha$ must be small. That is why we chose range of 0.01-0.05 as seen in Table 2. But one can still extend the table to other range say 0.06………..0.09 . $\alpha$ must lie in the range 0< $\alpha$ <1.

**Table 1:** Potential parameters of some selected diatomic molecules [20].

| Diatomic Molecules | $D_e(eV)$ | $r_e(\overset{o}{A})$ | $\mu(\overset{o}{A})$ |
|---|---|---|---|
| $H_2$ | 4.7446 | 0.7416 | 0.5039 |
| $CO$ | 10.845 | 1.1282 | 6.8606 |
| $NO$ | 8.0437 | 1.1508 | 7.4684 |
| $N_2$ | 11.938 | 1.0940 | 7.0034 |
| $Ar_2$ | 1.6720 | 2.5300 | 53.934 |

**Table 2:** Energy eigenvalue for $0.01 \le \alpha \le 0.05$

| | $\alpha$ | $H_2$ | $CO$ | $NO$ | $N_2$ | $Ar_2$ |
|---|---|---|---|---|---|---|
| $E_{nlm}(eV)$ | 0.01 | $-6.1310$ | $-10.183$ | $-8.8804$ | $-12.191$ | $-4.2942$ |
| | 0.02 | $-5.7632$ | $-7.3483$ | $-7.9872$ | $-8.7922$ | $-3.6548$ |
| | 0.03 | $-5.5244$ | $-6.7375$ | $-6.8755$ | $-7.3482$ | $-3.3075$ |
| | 0.04 | $-5.0912$ | $-6.1143$ | $-5.8349$ | $-6.5159$ | $-3.0981$ |
| | 0.05 | $-4.9396$ | $-4.9992$ | $-5.0399$ | $-6.0141$ | $-2.9621$ |

### 3.0 Hellmann-Feynman Theorem (HFT) in angle dependent Yukawa potential

The Hamiltonian which contains the effective potential with respect to the radial part of Eq.(2)can be express as

$$H=-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}-\frac{V_0}{r}+V_0\alpha r \qquad (14)$$

With the help of this equation one can evaluate the required expectation values of interest.

### 3.1 Expectation value equation for $<r^{-2}>$ and $<r^{-1}>$

The energy for the radial part is given in equation (7). Taking the derivative of Eq. (7) with respect to $l$ (orbital angular quantum number) gives

$$\frac{\partial E_{nl}}{\partial l}=\frac{4\mu V_0^2(2l+1)}{\hbar^2\left[\sqrt{l(l+1)+\frac{1}{4}}\right]\left[(2n+1)+2\sqrt{l(l+1)+\frac{1}{4}}\right]^3} \tag{15}$$

Differentiating equation (14) with respect $l$ gives

$$\frac{\partial H(l)}{\partial l}=-\frac{\hbar^2(2l+1)}{2\mu}<r^{-2}> \tag{16}$$

Using HFT then, equating Eq. (15) to (16) gives

$$\frac{\partial E_n(l)}{\partial l}=\langle\Psi(l)|\frac{\partial H(l)}{\partial l}|\Psi(l)\rangle\Rightarrow-\frac{\hbar^2(2l+1)}{2\mu}<r^{-2}>=\frac{4\mu V_0^2(2l+1)}{\hbar^2\left[\sqrt{l(l+1)+\frac{1}{4}}\right]\left[(2n+1)+2\sqrt{l(l+1)+\frac{1}{4}}\right]^3}$$

$$\Rightarrow<r^{-2}>=\frac{8\mu V_0^2}{\hbar^4\left[\sqrt{l(l+1)+\frac{1}{4}}\right]\left[(2n+1)+2\sqrt{l(l+1)+\frac{1}{4}}\right]^3} \tag{17}$$

Equation (17) gives the expectation value equation for $<r^{-2}>$.
Also taking the partial derivative of equation (7) with respect to $V_0$ gives

$$\frac{\partial E_{nl}}{\partial V_0}=\alpha-\frac{4\mu V_0}{\hbar^2\left[(2n+1)+2\sqrt{l(l+1)+\frac{1}{4}}\right]^2} \tag{18}$$

Taking the derivative of equation (14) with respect to $V_0$ gives

$$\frac{\partial H}{\partial V_0}=-\frac{1}{r}+\alpha r. \tag{19}$$

Equating equation (19) to (18) with respect to HFT gives

$$\frac{\partial E_n(V_0)}{\partial V_0}=\langle\Psi(V_0)|\frac{\partial H(V_0)}{\partial V_0}|\Psi(V_0)\rangle$$

$$\Rightarrow<r^{-1}>=\alpha(r-1)+\frac{4\mu V_0}{\hbar^2\left[(2n+1)+2\sqrt{l(l+1)+\frac{1}{4}}\right]^2} \tag{20}$$

### 3.2 Expectation value equation for $<T>$ and $<p^2>$

In this section, we shall evaluate the expectation values for kinetic energy $<T>$ and momentum squared $<p^2>$. Taking the partial derivative of equation (7) with respect to $\mu$ gives

$$\frac{\partial E_{nl}}{\partial\mu}=-\frac{2V_0^2}{\hbar^2\left[(2n+1)+2\sqrt{l(l+1)+\frac{1}{4}}\right]^2} \tag{21}$$

However, the Hamiltonian expressed in terms of $\mu$ is

$$\left\langle \Psi(\mu)\right| \frac{\partial H(\mu)}{\partial \mu} \left|\Psi(\mu)\right\rangle = -\frac{\hbar^2}{2\mu^2}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu^2}\frac{l(l+1)}{r^2} = \frac{1}{\mu}\left( -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu^2}\frac{l(l+1)}{r^2} \right)$$

$$\left\langle \Psi(\mu)\right| \frac{\partial H(\mu)}{\partial \mu} \left|\Psi(\mu)\right\rangle = -\frac{1}{\mu}\left( \frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu^2}\frac{l(l+1)}{r^2} \right) \Rightarrow -\frac{1}{\mu}\left(H - V\right) = -\frac{1}{\mu} < T >$$

$$\Rightarrow \left\langle \Psi(\mu)\right| \frac{\partial H(\mu)}{\partial \mu} \left|\Psi(\mu)\right\rangle = -\frac{1}{\mu} < T > \tag{22}$$

Equating equation (21) to (22) gives

$$< T > = \frac{2\mu V_0^2}{\hbar^2 \left[ \left(2n+1\right) + 2\sqrt{l(l+1) + \frac{1}{4}} \right]^2} \tag{23}$$

The relationship between kinetic energy and momentum is given as

$$T = \frac{p^2}{2\mu} \tag{24}$$

Substituting equation (24) into (22) gives

$$\left\langle \Psi(\mu)\right| \frac{\partial H(\mu)}{\partial \mu} \left|\Psi(\mu)\right\rangle = -\frac{1}{\mu} < \frac{p^2}{2\mu} > \Rightarrow -\frac{1}{2\mu^2} < p^2 > \tag{25}$$

Equating equation (21) to (25) gives the expectation value for $< p^2 >$ as

$$< p^2 > = \frac{4\mu^2 V_0^2}{\hbar^2 \left[ \left(2n+1\right) + 2\sqrt{l(l+1) + \frac{1}{4}} \right]^2} \tag{26}$$

## 4.0 Calculation of expectation value for the total effective potential.

However, the total energy equation which comprises of the radial part and the angular part is given in Eq. (11). In this case the Hamiltonian incorporating the effective potential is given as

$$H = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{V_0(1-\alpha r)}{r} + \frac{\hbar^2}{2\mu}\frac{V_0(\theta)}{r^2} \tag{27}$$

Taking the derivative of equation (11) with respect to $\mu$ gives

$$\frac{\partial E_{nl}}{\partial V_0} = -\frac{2V_0^2}{\hbar^2 \left[ \left(2n+1\right) + 2\delta \right]^2} \tag{28}$$

Where

$$\delta = \sqrt{ 4\left(n + \frac{1}{2}\right)^2 + 2\left(2n+1\right)\left( \sqrt{m^2 + \gamma + \beta + \eta} + \sqrt{\gamma + \frac{1}{4}} \right) + 2\sqrt{\left(m^2 + \gamma + \beta + \eta\right)\left(\gamma + \frac{1}{4}\right)} + m^2 + 2\gamma + \beta + \frac{1}{4} }$$

Then using HFT,

$$\begin{aligned} -\frac{1}{\mu} < T > &= -\frac{2V_0^2}{\hbar^2 \left[ \left(2n+1\right) + 2\delta \right]^2} \\ \Rightarrow < T > &= \frac{2\mu V_0^2}{\hbar^2 \left[ \left(2n+1\right) + 2\delta \right]^2} \end{aligned} \tag{29}$$

Also, using the same principle,

$$-\frac{1}{\mu}<\frac{p^2}{2\mu}>=-\frac{2V_0^2}{\hbar^2\left[\left(2n+1\right)+2\delta\right]^2}$$
$$\Rightarrow<p^2>=\frac{4\mu^2V_0^2}{\hbar^2\left[\left(2n+1\right)+2\delta\right]^2} \quad (30)$$

## 5.0 Results and Discussion

From the radial energy eigenvalues result of Eq.(7), we have applied the HFT to evaluate the expression for $<r^{-2}>$, $<r^{-1}>$, $<T>$ and $<p^2>$**.** While the total effective energy of the system(comprises of the radial part and the angular part) of Eq.(11) was used to obtain expectation values of $<T>$ and $<p^2>$ for total effective potential for the five selected diatomic molecules $H_2, CO, NO, N_2$ and $Ar_2$ .

The spectroscopic constants of these diatomic molecules are given in Table () taken from ref.[16]. The numeriacal values of $<r^{-2}>$ for the diatomic molecules $H_2, CO, NO, N_2$ and $Ar_2$ are presented in Tables 3,4,5,6 and 7 respectively while that of $<r^{-1}>$ for $H_2, CO, NO, N_2$ and $Ar_2$ are discussed in Tables 8,9,10,11 and 12 respectively.

In Tables 13-17 , we have discussed the numerical simulations of $<T>$ for these diatomic molecules under consideration. While the numerical results of $<p^2>$ for these molecules are discussed in Tables 18 and 22 all for the radial case. For the effective potential, the numerical discussions for $<T>$ and $<p^2>$ are presented in Tables 23, 24,25, and 26 respectively.

It must be noted that a bound state energy could be negative (in this situation we are discussing particle case of the system) and positive (this is a case of antiparticle description of the system). In this our work from Tables 3-12 we are having negative values for the $<r^{-2}>$ and $<r^{-1}>$ and this suggest the bound state status for the particles. From Tables 13-22, though the same radial system the expectation values for $<T>$ and $<p^2>$ are positive. In Tables 23-26 where we are dealing with the effective potential ( combination of both the radial and angular parts), it is noticed that positives values for the expectation values for the $<T>$ and $<p^2>$ are obtained which indicate description for the antiparticles of this system.

**Table 3: Expectation values of $<r^{-2}>$ for $H_2$ molecule**

| $n$ | $l$ | $<r^{-2}>_{nl}\,(\dot{A}^{-2})\times10^{-3}$ | $n$ | $l$ | $<r^{-2}>_{nl}\,(\dot{A}^{-2})\times10^{-5}$ | $n$ | $l$ | $<r^{-2}>_{nl}\,(\dot{A}^{-2})\times10^{-5}$ | $n$ | $l$ | $<r^{-2}>_{nl}\,(\dot{A}^{-2})\times10^{-6}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -0.20313217 | **0** | **1** | -0.84638403 | **0** | **2** | -0.84638403 | **0** | **3** | -0.45342002 |
| **1** | **0** | -0.02539152 | **1** | **1** | -0.25078045 | **1** | **2** | -0.06347880 | **1** | **3** | -0.23215105 |
| **2** | **0** | -0.0075234 | **2** | **1** | -0.10579800 | **2** | **2** | -0.03250114 | **2** | **3** | -0.13434667 |
| **3** | **0** | -0.00317394 | **3** | **1** | -0.54168578 | **3** | **2** | -0.01880853 | **3** | **3** | -0.08460315 |
| **4** | **0** | -0.00162505 | **4** | **1** | -0.03134755 | **4** | **2** | -0.01184444 | **4** | **3** | -0.05667750 |
| **5** | **0** | -0.0009404 | **5** | **1** | -0.01974073 | **5** | **2** | -0.00793485 | **5** | **3** | -0.03980642 |
| **6** | **0** | -0.00592222 | **6** | **1** | -0.01322475 | **6** | **2** | -0.00557289 | **6** | **3** | -0.02901888 |
| **7** | **0** | -0.00396742 | **7** | **1** | -0.00928816 | **7** | **2** | -0.00406264 | **7** | **3** | -0.02180231 |
| **8** | **0** | -0.00278644 | **8** | **1** | -0.00677107 | **8** | **2** | -0.00305232 | **8** | **3** | -0.01679333 |

**Table 4: Expectation values of $< r^{-2} >$ For CO Molecule**

| $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-1}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-2}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-2}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-4}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -0.37654266 | **0** | **1** | -0.15689277 | **0** | **2** | -0.15689277 | **0** | **3** | -0.84049701 |
| **1** | **0** | -0.04706783 | **1** | **1** | -0.04648674 | **1** | **2** | -0.01176695 | **1** | **3** | -0.43033447 |
| **2** | **0** | -0.01394602 | **2** | **1** | -0.01961159 | **2** | **2** | -0.00602468 | **2** | **3** | -0.24903615 |
| **3** | **0** | -0.00588347 | **3** | **1** | -0.01004113 | **3** | **2** | -0.00348650 | **3** | **3** | -0.15682743 |
| **4** | **0** | -0.00301234 | **4** | **1** | -0.00581084 | **4** | **2** | -0.00219558 | **4** | **3** | -0.10506213 |
| **5** | **0** | -0.00174325 | **5** | **1** | -0.00365930 | **5** | **2** | -0.00147086 | **5** | **3** | -0.07378848 |
| **6** | **0** | -0.00109779 | **6** | **1** | -0.00245144 | **6** | **2** | -0.00103303 | **6** | **3** | -0.05379180 |
| **7** | **0** | -0.00073543 | **7** | **1** | -0.00172173 | **7** | **2** | -0.00075308 | **7** | **3** | -0.04041458 |
| **8** | **0** | -0.00051651 | **8** | **1** | -0.00125514 | **8** | **2** | -0.00056580 | **8** | **3** | -0.03112951 |

**Table 5: Expectation values of $< r^{-2} >$ for NO molecule**

| $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-1}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-2}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-2}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-4}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -0.44621599 | **0** | **1** | -0.18592333 | **0** | **2** | -0.18592333 | **0** | **3** | -0.99601783 |
| **1** | **0** | -0.05577699 | **1** | **1** | -0.05508839 | **1** | **2** | -0.01394425 | **1** | **3** | -0.50996113 |
| **2** | **0** | -0.01652651 | **2** | **1** | -0.02324041 | **2** | **2** | -0.00071394 | **2** | **3** | -0.29511639 |
| **3** | **0** | - 0.006972123 | **3** | **1** | -0.01189909 | **3** | **2** | -0.00041316 | **3** | **3** | -0.18584589 |
| **4** | **0** | -0.00356972 | **4** | **1** | -0.00068860 | **4** | **2** | -0.00026018 | **4** | **3** | -0.12450223 |
| **5** | **0** | -0.00206581 | **5** | **1** | -0.00043364 | **5** | **2** | -0.00017430 | **5** | **3** | -0.08744189 |
| **6** | **0** | -0.00130092 | **6** | **1** | -0.00029050 | **6** | **2** | -0.00012241 | **6** | **3** | -0.06374514 |
| **7** | **0** | -0.00087151 | **7** | **1** | -0.00020403 | **7** | **2** | -0.00089243 | **7** | **3** | -0.04789266 |
| **8** | **0** | -0.00061209 | **8** | **1** | -0.00014873 | **8** | **2** | -0.00067049 | **8** | **3** | -0.036889549 |

**Table 6: Expectation values of $< r^{-2} >$ for $N_2$ molecule**

| $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-1}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-2}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-2}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-4}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -0.39238089 | **0** | **1** | -0.16349204 | **0** | **2** | -0.16349204 | **0** | **3** | -0.87585021 |
| **1** | **0** | -0.04904761 | **1** | **1** | -0.00484420 | **1** | **2** | -0.01226190 | **1** | **3** | -0.44843531 |
| **2** | **0** | -0.01453262 | **2** | **1** | -0.00204365 | **2** | **2** | -0.00627809 | **2** | **3** | -0.25951117 |
| **3** | **0** | -0.00613095 | **3** | **1** | -0.00104634 | **3** | **2** | -0.00363315 | **3** | **3** | -0.16342395 |
| **4** | **0** | -0.00313904 | **4** | **1** | -0.00060552 | **4** | **2** | -0.00022879 | **4** | **3** | -0.10948128 |
| **5** | **0** | -0.00181657 | **5** | **1** | -0.00038132 | **5** | **2** | -0.00015327 | **5** | **3** | -0.07689219 |
| **6** | **0** | -0.00114396 | **6** | **1** | -0.00025545 | **6** | **2** | -0.00010764 | **6** | **3** | -0.05605441 |
| **7** | **0** | -0.00076636 | **7** | **1** | -0.00017941 | **7** | **2** | -0.00078476 | **7** | **3** | -0.04211451 |
| **8** | **0** | -0.00053824 | **8** | **1** | -0.00013079 | **8** | **2** | -0.00058960 | **8** | **3** | -0.03243889 |

**Table 7: Expectation values of $< r^{-2} >$ for $Ar_2$ molecule**

| $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-1}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-1}$ | $n$ | $l$ | $< r^{-2} >_{nl}\ (\dot{A}^{-2})\times 10^{-2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -2.32710110 | **0** | **1** | -0.96962545 | **0** | **2** | -0.96962545 | **0** | **3** | -0.51944221 |
| **1** | **0** | -0.29088764 | **1** | **1** | -0.28729643 | **1** | **2** | -0.07272190 | **1** | **3** | -0.26595441 |
| **2** | **0** | -0.08618892 | **2** | **1** | -0.12120318 | **2** | **2** | -0.037233617 | **2** | **3** | -0.15390880 |
| **3** | **0** | -0.03636095 | **3** | **1** | -0.06205602 | **3** | **2** | -0.02154723 | **3** | **3** | -0.09692216 |
| **4** | **0** | -0.01861680 | **4** | **1** | -0.03591205 | **4** | **2** | -0.01356910 | **4** | **3** | -0.06493027 |
| **5** | **0** | -0.01077361 | **5** | **1** | -0.02261517 | **5** | **2** | -0.09090238 | **5** | **3** | -0.04560260 |
| **6** | **0** | -0.00678455 | **6** | **1** | -0.01515039 | **6** | **2** | -0.06384365 | **6** | **3** | -0.03324430 |
| **7** | **0** | -0.00454511 | **7** | **1** | -0.01064060 | **7** | **2** | -0.04654202 | **7** | **3** | -0.02497693 |
| **8** | **0** | -0.00319218 | **8** | **1** | -0.07757003 | **8** | **2** | -0.03496771 | **8** | **3** | -0.01923860 |

**Table 8: Expectation values of $< r^{-1} >$ for H$_2$ molecule**

| $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.00027800 | **0** | **1** | -0.00728050 | **0** | **2** | -0.00868022 | **0** | **3** | -0.00917012 |
| **1** | **0** | -0.00728050 | **1** | **1** | -0.00868022 | **1** | **2** | -0.00917012 | **1** | **3** | -0.00939688 |
| **2** | **0** | -0.00868022 | **2** | **1** | -0.00917012 | **2** | **2** | -0.00939688 | **2** | **3** | -0.00952005 |
| **3** | **0** | -0.00917012 | **3** | **1** | -0.00939688 | **3** | **2** | -0.00980000 | **3** | **3** | -0.00959432 |
| **4** | **0** | -0.00939688 | **4** | **1** | -0.00019238 | **4** | **2** | -0.00959432 | **4** | **3** | -0.00964253 |
| **5** | **0** | -0.00980000 | **5** | **1** | -0.00959432 | **5** | **2** | -0.00964253 | **5** | **3** | -0.00967558 |
| **6** | **0** | -0.00959432 | **6** | **1** | -0.00964253 | **6** | **2** | -0.00967558 | **6** | **3** | -0.00969922 |
| **7** | **0** | -0.00964253 | **7** | **1** | -0.00967558 | **7** | **2** | -0.00980000 | **7** | **3** | -0.00971671 |
| **8** | **0** | -0.00967558 | **8** | **1** | -0.00969922 | **8** | **2** | -0.00971671 | **8** | **3** | -0.00973001 |

**Table 9: Expectation values of $< r^{-1} >$ for CO Molecule**

| $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -0.12741200 | **0** | **1** | 0.02450300 | **0** | **2** | -0.00544577 | **0** | **3** | -0.00122425 |
| **1** | **0** | -0.02450300 | **1** | **1** | 0.0054457 | **1** | **2** | -0.00122425 | **1** | **3** | -0.00431152 |
| **2** | **0** | -0.00544577 | **2** | **1** | -0.0012242 | **2** | **2** | -0.00431152 | **2** | **3** | -0.00598855 |
| **3** | **0** | -0.0012242 | **3** | **1** | -0.0043115 | **3** | **2** | -0.00980000 | **3** | **3** | -0.00699975 |
| **4** | **0** | -0.0043115 | **4** | **1** | -0.0001923 | **4** | **2** | -0.00699975 | **4** | **3** | -0.00765606 |
| **5** | **0** | -0.0098000 | **5** | **1** | -0.0069997 | **5** | **2** | -0.00765606 | **5** | **3** | -0.00810602 |
| **6** | **0** | -0.0069997 | **6** | **1** | -0.0076560 | **6** | **2** | -0.00810602 | **6** | **3** | -0.00842788 |
| **7** | **0** | -0.0076560 | **7** | **1** | -0.0081060 | **7** | **2** | -0.00980000 | **7** | **3** | -0.00866601 |
| **8** | **0** | -0.0081060 | **8** | **1** | -0.0084278 | **8** | **2** | -0.00866601 | **8** | **3** | -0.0088471 |

**Table 10: Expectation values of $< r^{-1} >$ for NO molecule**

| $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})\times 10^{-2}$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})\times 10^{-2}$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})\times 10^{-2}$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})\times 10^{-2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -0.00139568 | **0** | **1** | -0.02754200 | **0** | **2** | -0.67964444 | **0** | **3** | -0.00000464 |
| **1** | **0** | - 0.02754200 | **1** | **1** | -0 .00679644 | **1** | **2** | -0.04645000 | **1** | **3** | -0.38252800 |
| **2** | **0** | -0.67964444 | **2** | **1** | -0.04645000 | **2** | **2** | -0.38252800 | **2** | **3** | -0.56508889 |
| **3** | **0** | -0.46450000 | **3** | **1** | -0.38252800 | **3** | **2** | -0.98000000 | **3** | **3** | -0.67516735 |
| **4** | **0** | -0.38252800 | **4** | **1** | -0.01923860 | **4** | **2** | -0.67516735 | **4** | **3** | -0.74661250 |
| **5** | **0** | -0.98000000 | **5** | **1** | -0.67516735 | **5** | **2** | -0.74661250 | **5** | **3** | -0.79559506 |
| **6** | **0** | -0.67516735 | **6** | **1** | -0.74661250 | **6** | **2** | -0.79559506 | **6** | **3** | -0.83063200 |
| **7** | **0** | -0.74661250 | **7** | **1** | -0.79559506 | **7** | **2** | -0.98000000 | **7** | **3** | -0.85655537 |
| **8** | **0** | -0.79559506 | **8** | **1** | -0.83063200 | **8** | **2** | -0.85655537 | **8** | **3** | -0.87627222 |

**Table 11: Expectation values of $< r^{-1} >$ for N$_2$ molecule**

| $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})\times 10^{-2}$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})\times 10^{-2}$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})\times 10^{-2}$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})\times 10^{-2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -0.00130268 | **0** | **1** | -0.02521700 | **0** | **2** | -0.57631111 | **0** | **3** | -0.10457500 |
| **1** | **0** | - 0.02521700 | **1** | **1** | -0.57631111 | **1** | **2** | -0.10457500 | **1** | **3** | -0.41972800 |
| **2** | **0** | -0.57631111 | **2** | **1** | -0.10457500 | **2** | **2** | -0.41972800 | **2** | **3** | -0.59092222 |
| **3** | **0** | -0.10457500 | **3** | **1** | -0.41972800 | **3** | **2** | -0.98000000 | **3** | **3** | -0.69414694 |
| **4** | **0** | -0.41972800 | **4** | **1** | -0.019238600 | **4** | **2** | -0.69414694 | **4** | **3** | -0.76114375 |
| **5** | **0** | -0.98000000 | **5** | **1** | -0.69414694 | **5** | **2** | -0.76114375 | **5** | **3** | -0.80707654 |
| **6** | **0** | -0.69414694 | **6** | **1** | -0.76114375 | **6** | **2** | -0.80707654 | **6** | **3** | -0.83993200 |
| **7** | **0** | -0.76114375 | **7** | **1** | -0.80707654 | **7** | **2** | -0.98000000 | **7** | **3** | -0.86424132 |
| **8** | **0** | -0.80707654 | **8** | **1** | -0.83993200 | **8** | **2** | -0.86424132 | **8** | **3** | -0.88273056 |

**Table 12: Expectation values of $< r^{-1} >$ for $Ar_2$ molecule**

| $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ | $n$ | $l$ | $< r^{-1} >_{nl}\ (\dot{A}^{-1})$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | -1.0688800 | **0** | **1** | -0.25987000 | **0** | **2** | -0.11005333 | **0** | **3** | -0.05761750 |
| **1** | **0** | -0.25987000 | **1** | **1** | - 0.11005330 | **1** | **2** | - 0.05761750 | **1** | **3** | -0.03334720 |
| **2** | **0** | - 0.11005333 | **2** | **1** | -0.05761750 | **2** | **2** | -0.03334720 | **2** | **3** | -0.02016333 |
| **3** | **0** | -0.05761750 | **3** | **1** | -0.03334720 | **3** | **2** | -0.00980000 | **3** | **3** | -0.01221387 |
| **4** | **0** | -0.03334720 | **4** | **1** | -0.00019238 | **4** | **2** | -0.01221387 | **4** | **3** | -0.00705437 |
| **5** | **0** | -0.00980000 | **5** | **1** | -0.01221387 | **5** | **2** | -0.00705437 | **5** | **3** | -0.00351703 |
| **6** | **0** | -0.01221387 | **6** | **1** | - 0.00705437 | **6** | **2** | -0.00351703 | **6** | **3** | -0.00098680 |
| **7** | **0** | -0.00705437 | **7** | **1** | -0.00351703 | **7** | **2** | -0.00980000 | **7** | **3** | -0.00088528 |
| **8** | **0** | -0.00351703 | **8** | **1** | - 0.00098680 | **8** | **2** | -0.00088528 | **8** | **3** | -0.00230916 |

**Table 13: Expectation values of $< T >$ for $H_2$ molecule**

| $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-3}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-4}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-4}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-5}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.10078000 | **0** | **1** | 0.25195000 | **0** | **2** | 0.11197777 | **0** | **3** | 0.62987500 |
| **1** | **0** | 0.01119777 | **1** | **1** | 0.11197777 | **1** | **2** | 0.06298750 | **1** | **3** | 0.40312000 |
| **2** | **0** | 0.01100533 | **2** | **1** | 0.06298750 | **2** | **2** | 0.04031200 | **2** | **3** | 0.27994444 |
| **3** | **0** | 0.00629875 | **3** | **1** | 0.04031200 | **3** | **2** | 0.02799444 | **3** | **3** | 0.20567346 |
| **4** | **0** | 0.00403120 | **4** | **1** | 0.02799444 | **4** | **2** | 0.02056734 | **4** | **3** | 0.15746875 |
| **5** | **0** | 0.00279944 | **5** | **1** | 0.02056734 | **5** | **2** | 0.01574687 | **5** | **3** | 0.12441975 |
| **6** | **0** | 0.00205673 | **6** | **1** | 0.01574687 | **6** | **2** | 0.01244197 | **6** | **3** | 0.10078000 |
| **7** | **0** | 0.00157468 | **7** | **1** | 0.01244197 | **7** | **2** | 0.01007800 | **7** | **3** | 0 .08328925 |
| **8** | **0** | 0.00124419 | **8** | **1** | 0.01007800 | **8** | **2** | 0.00832892 | **8** | **3** | 0.06998611 |

**Table 14: Expectation values of $< T >$ for CO molecule**

| $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-2}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-3}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-3}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-4}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.13721200 | **0** | **1** | 0.34303000 | **0** | **2** | 0.15245778 | **0** | **3** | 0.85757500 |
| **1** | **0** | 0.01524577 | **1** | **1** | 0.15245778 | **1** | **2** | 0.08575750 | **1** | **3** | 0.54884800 |
| **2** | **0** | 0.11005333 | **2** | **1** | 0.08575750 | **2** | **2** | 0.05488480 | **2** | **3** | 0.38114444 |
| **3** | **0** | 0.00857575 | **3** | **1** | 0.05488480 | **3** | **2** | 0.03811444 | **3** | **3** | 0.28002449 |
| **4** | **0** | 0.00548848 | **4** | **1** | 0.03811444 | **4** | **2** | 0.02800244 | **4** | **3** | 0.21439375 |
| **5** | **0** | 0.00381144 | **5** | **1** | 0.02800244 | **5** | **2** | 0.02143937 | **5** | **3** | 0.16939753 |
| **6** | **0** | 0.00280024 | **6** | **1** | 0.02143937 | **6** | **2** | 0.01693975 | **6** | **3** | 0.13721200 |
| **7** | **0** | 0.00214393 | **7** | **1** | 0.01693975 | **7** | **2** | 0.01372120 | **7** | **3** | 0.11339835 |
| **8** | **0** | 0.00169397 | **8** | **1** | 0.01372120 | **8** | **2** | 0.01133983 | **8** | **3** | 0.09528611 |

**Table 15: Expectation values of $< T >$ for NO molecule**

| $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-2}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-3}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-4}$ | $n$ | $l$ | $< T >_{nl}\ (eV)\times10^{-4}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.14936800 | **0** | **1** | 0.37342000 | **0** | **2** | 0.16596444 | **0** | **3** | 0.93355000 |
| **1** | **0** | 0.01659644 | **1** | **1** | 0.16596444 | **1** | **2** | 0.93355000 | **1** | **3** | 0.59747200 |
| **2** | **0** | 0.11005333 | **2** | **1** | 0.09335500 | **2** | **2** | 0.59747200 | **2** | **3** | 0.41491111 |
| **3** | **0** | 0.00933550 | **3** | **1** | 0.05974720 | **3** | **2** | 0.41491111 | **3** | **3** | 0.30483265 |
| **4** | **0** | 0.00597472 | **4** | **1** | 0.04149111 | **4** | **2** | 0.30483265 | **4** | **3** | 0.23338750 |
| **5** | **0** | 0.00414911 | **5** | **1** | 0.03048326 | **5** | **2** | 0.23338750 | **5** | **3** | 0.18440494 |
| **6** | **0** | 0.00304832 | **6** | **1** | 0.02333875 | **6** | **2** | 0.18440494 | **6** | **3** | 0.14936800 |
| **7** | **0** | 0.00233387 | **7** | **1** | 0.01844049 | **7** | **2** | 0.14936800 | **7** | **3** | 0.12344463 |
| **8** | **0** | 0.00184404 | **8** | **1** | 0.01493680 | **8** | **2** | 0.12344463 | **8** | **3** | 0.10372778 |

**Table 16: Expectation values of $<T>$ for $N_2$ molecule**

| $n$ | $l$ | $<T>_{nl}\,(eV)\times10^{-2}$ | $n$ | $l$ | $<T>_{nl}\,(eV)\times10^{-3}$ | $n$ | $l$ | $<T>_{nl}\,(eV)\times10^{-3}$ | $n$ | $l$ | $<T>_{nl}\,(eV)\times10^{-4}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.14006800 | **0** | **1** | 0.35017000 | **0** | **2** | 0.15563111 | **0** | **3** | 0.87542500 |
| **1** | **0** | 0.01556311 | **1** | **1** | 0.15563111 | **1** | **2** | 0.08754250 | **1** | **3** | 0.56027200 |
| **2** | **0** | 0.00110053 | **2** | **1** | 0.08754250 | **2** | **2** | 0.05602720 | **2** | **3** | 0.38907778 |
| **3** | **0** | 0.00875425 | **3** | **1** | 0.05602720 | **3** | **2** | 0.03890777 | **3** | **3** | 0.28585306 |
| **4** | **0** | 0.00560272 | **4** | **1** | 0.03890777 | **4** | **2** | 0.02858530 | **4** | **3** | 0.21885625 |
| **5** | **0** | 0.00389077 | **5** | **1** | 0.02858530 | **5** | **2** | 0.02188562 | **5** | **3** | 0.17292346 |
| **6** | **0** | 0.00285853 | **6** | **1** | 0.02188562 | **6** | **2** | 0.01729234 | **6** | **3** | 0.14006800 |
| **7** | **0** | 0.00218856 | **7** | **1** | 0.01729234 | **7** | **2** | 0.01400680 | **7** | **3** | 0.11575868 |
| **8** | **0** | 0.00172923 | **8** | **1** | 0.01400680 | **8** | **2** | 0.01157586 | **8** | **3** | 0.97269444 |

**Table 17: Expectation values of $<T>$ for $Ar_2$ molecule**

| $n$ | $l$ | $<T>_{nl}\,(eV)$ | $n$ | $l$ | $<T>_{nl}\,(eV)\times10^{-2}$ | $n$ | $l$ | $<T>_{nl}\,(eV)\times10^{-2}$ | $n$ | $l$ | $<T>_{nl}\,(eV)\times10^{-3}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.01078680 | **0** | **1** | 0.26967000 | **0** | **2** | 0.11985333 | **0** | **3** | 0.67417500 |
| **1** | **0** | 0.00119853 | **1** | **1** | 0.11985332 | **1** | **2** | 0.06741750 | **1** | **3** | 0.43147200 |
| **2** | **0** | 0.11005333 | **2** | **1** | 0.06741750 | **2** | **2** | 0.04314720 | **2** | **3** | 0.29963333 |
| **3** | **0** | 0.00067417 | **3** | **1** | 0.04314720 | **3** | **2** | 0.02996333 | **3** | **3** | 0.22013878 |
| **4** | **0** | 0.00043147 | **4** | **1** | 0.02996333 | **4** | **2** | 0.02201387 | **4** | **3** | 0.16854375 |
| **5** | **0** | 0.00029963 | **5** | **1** | 0.02201387 | **5** | **2** | 0.01685437 | **5** | **3** | 0.13317037 |
| **6** | **0** | 0.00022013 | **6** | **1** | 0.01685437 | **6** | **2** | 0.01331703 | **6** | **3** | 0.10786800 |
| **7** | **0** | 0.00016854 | **7** | **1** | 0.01331703 | **7** | **2** | 0.01078680 | **7** | **3** | 0.08914710 |
| **8** | **0** | 0.00013317 | **8** | **1** | 0.01078680 | **8** | **2** | 0.00891471 | **8** | **3** | 0.07490833 |

**Table 18: Expectation values of $<P^2>$ for $H_2$ molecule**

| $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-3}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-4}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-4}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-5}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.10156608 | **0** | **1** | 0.25391521 | **0** | **2** | 0.11285120 | **0** | **3** | 0.63478802 |
| **1** | **0** | 0.01128512 | **1** | **1** | 0.11285120 | **1** | **2** | 0.06347880 | **1** | **3** | 0.40626434 |
| **2** | **0** | 0.11005333 | **2** | **1** | 0.06347880 | **2** | **2** | 0.04062643 | **2** | **3** | 0.28212801 |
| **3** | **0** | 0.00634788 | **3** | **1** | 0.04062643 | **3** | **2** | 0.02821280 | **3** | **3** | 0.20727772 |
| **4** | **0** | 0.00406264 | **4** | **1** | 0.02821280 | **4** | **2** | 0.02072777 | **4** | **3** | 0.15869701 |
| **5** | **0** | 0.00282128 | **5** | **1** | 0.02072777 | **5** | **2** | 0.01586970 | **5** | **3** | 0.12539023 |
| **6** | **0** | 0.00207277 | **6** | **1** | 0.01586970 | **6** | **2** | 0.01253902 | **6** | **3** | 0.10156608 |
| **7** | **0** | 0.00158697 | **7** | **1** | 0.01253902 | **7** | **2** | 0.01015660 | **7** | **3** | 0.08393891 |
| **8** | **0** | 0.00125390 | **8** | **1** | 0.01015660 | **8** | **2** | 0.00839389 | **8** | **3** | 0.07053200 |

**Table 19: Expectation values of $<p^2>$ for CO molecule**

| $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.01882713 | **0** | **1** | 0.47067832 | **0** | **2** | 0.20919037 | **0** | **3** | 0.11766958 |
| **1** | **0** | 0.00209190 | **1** | **1** | 0.20919037 | **1** | **2** | 0.11766958 | **1** | **3** | 0.07530853 |
| **2** | **0** | 0.11005333 | **2** | **1** | 0.11766958 | **2** | **2** | 0.07530853 | **2** | **3** | 0.05229759 |
| **3** | **0** | 0.00117669 | **3** | **1** | 0.07530853 | **3** | **2** | 0.05229759 | **3** | **3** | 0.03842272 |
| **4** | **0** | 0.00075308 | **4** | **1** | 0.05229759 | **4** | **2** | 0.03842272 | **4** | **3** | 0.02941739 |
| **5** | **0** | 0.00052297 | **5** | **1** | 0.03842272 | **5** | **2** | 0.02941739 | **5** | **3** | 0.02324337 |
| **6** | **0** | 0.00038422 | **6** | **1** | 0.02941739 | **6** | **2** | 0.02324337 | **6** | **3** | 0.01882713 |
| **7** | **0** | 0.00029417 | **7** | **1** | 0.02324337 | **7** | **2** | 0.01882713 | **7** | **3** | 0.0155596 |
| **8** | **0** | 0.00023243 | **8** | **1** | 0.01882713 | **8** | **2** | 0.01555961 | **8** | **3** | 0.01307439 |

**Table 20: Expectation values of $<p^2>$ for NO molecule**

| $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.02231079 | **0** | **1** | 0.55776999 | **0** | **2** | 0.24789777 | **0** | **3** | 0.13944250 |
| **1** | **0** | 0.00247897 | **1** | **1** | 0.24789777 | **1** | **2** | 0.13944250 | **1** | **3** | 0.08924319 |
| **2** | **0** | 0.11005333 | **2** | **1** | 0.13944250 | **2** | **2** | 0.08924319 | **2** | **3** | 0.06197444 |
| **3** | **0** | 0.00139442 | **3** | **1** | 0.08924319 | **3** | **2** | 0.06197444 | **3** | **3** | 0.04553224 |
| **4** | **0** | 0.00089243 | **4** | **1** | 0.06197444 | **4** | **2** | 0.04553224 | **4** | **3** | 0.03486062 |
| **5** | **0** | 0.00061974 | **5** | **1** | 0.04553224 | **5** | **2** | 0.03486062 | **5** | **3** | 0.02754419 |
| **6** | **0** | 0.00045532 | **6** | **1** | 0.03486062 | **6** | **2** | 0.02754419 | **6** | **3** | 0.02231079 |
| **7** | **0** | 0.00034860 | **7** | **1** | 0.02754419 | **7** | **2** | 0.02231079 | **7** | **3** | 0.01843867 |
| **8** | **0** | 0.00027544 | **8** | **1** | 0.02231079 | **8** | **2** | 0.01843867 | **8** | **3** | 0.01549361 |

**Table 21: Expectation values of $<p^2>$ for $N_2$ molecule**

| $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-2}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.01961904 | **0** | **1** | 0.49047612 | **0** | **2** | 0.21798938 | **0** | **3** | 0.12261903 |
| **1** | **0** | 0.00217989 | **1** | **1** | 0.21798938 | **1** | **2** | 0.12261903 | **1** | **3** | 0.07847617 |
| **2** | **0** | 0.11005333 | **2** | **1** | 0.12261903 | **2** | **2** | 0.07847617 | **2** | **3** | 0.05449734 |
| **3** | **0** | 0.00122619 | **3** | **1** | 0.07847617 | **3** | **2** | 0.05449734 | **3** | **3** | 0.04003886 |
| **4** | **0** | 0.00078476 | **4** | **1** | 0.05449734 | **4** | **2** | 0.04003886 | **4** | **3** | 0.03065475 |
| **5** | **0** | 0.00054497 | **5** | **1** | 0.04003886 | **5** | **2** | 0.03065475 | **5** | **3** | 0.02422104 |
| **6** | **0** | 0.00040038 | **6** | **1** | 0.03065475 | **6** | **2** | 0.02422104 | **6** | **3** | 0.01961904 |
| **7** | **0** | 0.00030654 | **7** | **1** | 0.02422104 | **7** | **2** | 0.01961904 | **7** | **3** | 0.01621408 |
| **8** | **0** | 0.00024221 | **8** | **1** | 0.01961904 | **8** | **2** | 0.01621408 | **8** | **3** | 0.01362433 |

**Table 22: Expectation values of $<p^2>$ for $Ar_2$ molecule**

| $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2$ | $n$ | $l$ | $<p^2>_{nl}\left(\frac{eV}{c}\right)^2\times10^{-1}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 1.16355050 | **0** | **1** | 0.29088764 | **0** | **2** | 0.12928339 | **0** | **3** | 0.72721909 |
| **1** | **0** | 0.12928339 | **1** | **1** | 0.12928339 | **1** | **2** | 0.07272190 | **1** | **3** | 0.46542022 |
| **2** | **0** | -3.8486397 | **2** | **1** | 0.07272190 | **2** | **2** | 0.04654202 | **2** | **3** | 0.32320848 |
| **3** | **0** | 0.07272190 | **3** | **1** | 0.04654202 | **3** | **2** | 0.03232084 | **3** | **3** | 0.23745929 |
| **4** | **0** | 0.04654202 | **4** | **1** | 0.03232084 | **4** | **2** | 0.02374592 | **4** | **3** | 0.18180477 |
| **5** | **0** | 0.03232084 | **5** | **1** | 0.02374592 | **5** | **2** | 0.01818047 | **5** | **3** | 0.14364822 |
| **6** | **0** | 0.02374592 | **6** | **1** | 0.01818047 | **6** | **2** | 0.01436482 | **6** | **3** | 0.11635505 |
| **7** | **0** | 0.01818047 | **7** | **1** | 0.01436482 | **7** | **2** | 0.01163550 | **7** | **3** | 0.09616120 |
| **8** | **0** | 0.01436482 | **8** | **0** | 0.01163550 | **8** | **0** | 0.00961612 | **8** | **0** | 0.08080212 |

**Table 23: Expectation values of $<T>(eV)$**

| $n$ | $l$ | $H_2$ | $n$ | $l$ | CO | $n$ | $l$ | **NO** |
|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.00001028 | **0** | **0** | 0.00014000 | **0** | **0** | 0.00015241 |
| **1** | **0** | 0.00000284 | **1** | **0** | 0.00003877 | **1** | **0** | 0.00004220 |
| **2** | **0** | 0.00000127 | **2** | **0** | 0.00001741 | **2** | **0** | 0.00001895 |
| **3** | **0** | 0.00000071 | **3** | **0** | 0.00000978 | **3** | **0** | 0.00001065 |
| **4** | **0** | 0.00000045 | **4** | **0** | 0.00000625 | **4** | **0** | 0.00000680 |
| **5** | **0** | 12.2996080 | **5** | **0** | 12.2996080 | **5** | **0** | 12.2996080 |
| **6** | **0** | 0.00000023 | **6** | **0** | 0.00000317 | **6** | **0** | 0.00000345 |
| **7** | **0** | 0.00000017 | **7** | **0** | 0.00000242 | **7** | **0** | 0.00000264 |
| **8** | **0** | 0.00000014 | **8** | **0** | 0.00000191 | **8** | **0** | 0.00000208 |

**Table 24: Expectation values of $<T>(eV)$**

| $n$ | $l$ | $N_2$ | $n$ | $l$ | $Ar_2$ |
|---|---|---|---|---|---|
| **0** | **0** | 0.00014292 | **0** | **0** | 0.00110067 |
| **1** | **0** | 0.00003958 | **1** | **0** | 0.00030481 |
| **2** | **0** | 0.00001777 | **2** | **0** | 0.00013689 |
| **3** | **0** | 0.00000999 | **3** | **0** | 0.00007696 |
| **4** | **0** | 0.00000638 | **4** | **0** | 0.00004914 |
| **5** | **0** | 12.2996080 | **5** | **0** | 12.2996080 |
| **6** | **0** | 0.00000324 | **6** | **0** | 0.00002496 |
| **7** | **0** | 0.00000247 | **7** | **0** | 0.00001907 |
| **8** | **0** | 0.00000195 | **8** | **0** | 0.00001504 |

**Table 25: Expectation values of $< p^2 >_{nl} \left(\frac{eV}{c}\right)^2$**

| $n$ | $l$ | $H_2$ | $n$ | $l$ | CO | $n$ | $l$ | **NO** |
|---|---|---|---|---|---|---|---|---|
| **0** | **0** | 0.00001036 | **0** | **0** | 0.00001036 | **0** | **0** | 0.00227656 |
| **1** | **0** | 0.00000287 | **1** | **0** | 0.00000287 | **1** | **0** | 0.00063045 |
| **2** | **0** | 0.00000128 | **2** | **0** | 0.00000128 | **2** | **0** | 0.00028313 |
| **3** | **0** | 0.00000072 | **3** | **0** | 0.00000072 | **3** | **0** | 0.00015918 |
| **4** | **0** | 0.00000046 | **4** | **0** | 0.00000046 | **4** | **0** | 0.00010164 |
| **5** | **0** | 12.2996080 | **5** | **0** | 12.2996080 | **5** | **0** | 12.2996080 |
| **6** | **0** | 0.00000023 | **6** | **0** | 0.00000023 | **6** | **0** | 0.00005162 |
| **7** | **0** | 0.00000017 | **7** | **0** | 0.00000017 | **7** | **0** | 0.00003945 |
| **8** | **0** | 0.00000014 | **8** | **0** | 0.00000014 | **8** | **0** | 0.00003112 |

**Table 26: Expectation values of $< p^2 >_{nl} \left(\frac{eV}{c}\right)^2$**

| $n$ | $l$ | $N_2$ | $n$ | $l$ | $Ar_2$ |
|---|---|---|---|---|---|
| **0** | **0** | 0.00200190 | **0** | **0** | 0.11872720 |
| **1** | **0** | 0.00055439 | **1** | **0** | 0.03287961 |
| **2** | **0** | 0.00024897 | **2** | **0** | 0.01476622 |
| **3** | **0** | 0.00013997 | **3** | **0** | 0.00830171 |
| **4** | **0** | 0.00008938 | **4** | **0** | 0.00530098 |
| **5** | **0** | 12.2996080 | **5** | **0** | 12.2996080 |
| **6** | **0** | 0.00004539 | **6** | **0** | 0.00269247 |
| **7** | **0** | 0.0000346 | **7** | **0** | 0.00205767 |
| **8** | **0** | 0.00002737 | **8** | **0** | 0.00162329 |

## 5.0 CONCLUSION

In this paper, we have applied the Hellmann-Feynmann theorem to calculate the expectation values of the Yukawa-angle dependent potential from the already obtained bound state solutions in ref. [16] . The expectation values $\langle r^{-2}\rangle$ , $\langle r^{-1}\rangle$ , $\langle T\rangle$ and $\langle p^{2}\rangle$ have been obtained numerically for diatomic molecules under investigation such as $H_2, CO, NO, N_2$ and $Ar_2$ for both the radial part of our system and the effective potential ( combined radial and angular parts). These results could be used to study the interactions of the noncentral potential for diatomic molecules.

## REFERENCES

[1] Wallace, D. B. (2004). A master of Science Thesis submitted to the Department of Mathematics, College of Art and Sciences, University of Central Florida, Orlando, Florida.

[2] Feynmann, R. P. (1939). Phys. Rev. 56, 340.

[3] Esteve, J. G. (2009). Generalization of the Hellmann-Feynmann theorem. arXiv: 0912.4153v1[quant-ph] 21 Dec 2009.

[4] Zhang, X. A; Chen, K. and Duan, Z. L. (2005) Chinese physics. **14**, 42

[5] Dong, S. H; Sun, G. H. and Lozada-Cassou, M. (2005) *Physical Letter*. A328, 299.

[6] Chen. C. Y. and Dong, S. H. (2005) *Physical Letter*. A335, 374.
[7] Alhaidari, A. D. (2005) Solution of relativistic Dirac-Hulthen problems. Journal of Physics and Mathematics. Gen 38, 3409.
[8] Zhang, M. C. and Wang, Z. B. (2005) *Chinese Physical Letter*. 22, 2994.
[9] Roy, A. K. (2004) The generalized pseuduspectral approach to the bound state of the Hulthen and Yukawa potentials. *Indian Journal of Physics*. Vol.65 No.1 pp. 1-15
[10] Yukalov, V; Yukalova, E. and Oliveira, F. (1998). Renormaliziation group solutions for Yukawa potential. *Journal of Physics*. A31, 4337-4348.
[11] Hamzavi, M; Movahedi, M; Thylwe, K-E and Rajabi, A. (2012) Approximate analytical solution of Yukawa Potential with arbituary angular momenta. *Chinese Physics Letter*. Vol. 29 No.8
[12] Hamzavi, M. and Ikhdair, S. M. (2013) Relativistic symmetries of fermions in the background of inverse quadratic Yukawa potential as a tensor. *Canadian Journal of Physics*. A36, 11807-11818.
[13] Ita, B; Ikot, A; Ikeuba, A. and Ebiekpe, V. (2014) Exact solution of Schrödinger equation for the Inverse quadratic Yukawa potential using Nikiforov-Uvarov method. *Journal of Theoretical Physics and Cryptography*. Vol.5, pp.7-11
[14] Alhaidari, A; Bahlouli, H; Nasser, I; and Abdelmonem, M. (2008) an efficient mapped pseudospectral method for weakly bound state. *Journal of Chemical Physics*. A41, 032001
[15] Ikhdair, S. M. and Sever, R. (2010) Approximate analytical solutions of the general Wood-Saxon potential including the Spin-orbit coupling term and spin symmetry. *Central European Journal of Physics*. Vol.5, 2322-3138
[13] Antia, A. D; Umo, E. A. and Umoren, C. C. (2015) solution of nonrelativistic Schrödinger equation with Hulthen-Yukawa plus ange dependent potential within the framework of Nikiforov-Uvarov method. *Journal of Theoretical Physics and Cryptography*. Vol.10, pp.1-8
[14] Yasuk, F; Durmus, A. and Boztosun, I. (2006) Exact analytical solution to the relativistic Klien-Gordon equation with a noncentral equal scalar and vector potentials. *Journal of Mathematics and Physics*. 49, 082302
[15] Hamzavi, M. and Rajabi, A. A. (2011) Exact solution of Dirac equation with Coulomb plus a novel angle dependent potential. *Z. Naturforsch*. 66a, 533
[16] Antia, A. D. and Akpan, O. P. (2017). Applied and Computational Mathematics 6(1), 54-59.
[17] Nikiforov, A. F. and Uvarov, V. B. (1988) *Special Functions of Mathematical Physics*. Basel: Birkhauser
[18] Tezcan, C. and Sever, R. (2009) A general approach of the exact solution of the Schrödinger equation. *International Journal of Theoretical Physics*. 48, 339
[19] Akcay, H. and Sever, R. (2011) Analytical solutions of schrodinger equation for the diatomic molecular potential with any angular potential. *Journal of molecular Structure: Theochem*. 845, 133
[20] Castro, E; Paz, J. and Martin, P. (2006) *Journal of molecular Structure: Theochem*. 46, 1122.