IRSTI 29.17.15 https://doi.org/10.26577/RCPh.2024.v91.i4.a10

A.H. Cacan*, B.A. Mamedov
Tokat Gaziosmanpasa University, Tokat, Turkey
*e-mail: aslihan.cacan@gop.edu.tr

AN ACCURATE AND EFFICIENT THEORETICAL ASSESSMENT OF THE THERMODYNAMIC PROPERTIES OF NON-POLAR GASES

Investigation of the intermolecular interactions and thermodynamic properties of real nonpolar gases is of high importance and can be evaluated through virial equation of state. A new, practical and general analytical method is obtained for the evaluation of the second virial coefficient (SVC) with Morse potential, which is significant for the investigation of all thermodynamic properties of gases. The first derivative of SVC with Morse potential analytical formulae is also established since it appears in the thermodynamic expressions. One of the significances of obtained formulae is their validity of all ranges of parameters providing accurate and precise results quickly. The accuracy of the applied method is tested by the calculations of SVC of Ne gas for a wide temperature range with both experimental and analytical data for comparison and Boyle temperature (T_B) of He, Ne, Ar, Kr, Xe, H_2, N_2, and O_2 gases with included highly accurate corresponding literature data for the comparison and proved to be consistent. In this study, we also used the acquired analytical formulae to obtain the changes in entropy, enthalpy, internal energy and free energy per pressure for the gases of He, Ne, Ar, Kr, Xe, H_2, N_2, and O_2. The results of $(\Delta S)/P$, $\Delta H/P$, $\Delta E/P$ and $\Delta F/P$ are compared with literature data that utilizes most commonly used potential Lennard-Jones (12-6) to acquire thermodynamic properties of gases for SVC calculations. The results proved that including previously ignored higher order term in the $(\Delta S)/P$ formula improved accuracy but still can be disregarded due to small contributions.

Keywords: Morse potential, second virial coefficient, thermodynamic properties.

А.Х. Чачан*, Б.А. Мамедов
Токат Газиосманпаша университеті, Токат қ., Түркия
*e-mail: aslihan.cacan@gop.edu.tr

Полярлы емес газдардың термодинамикалық қасиеттерін дәл және тиімді теориялық бағалау

Нақты полярлы емес газдардың молекулааралық әрекеттесулері мен термодинамикалық қасиеттерін зерттеудің маңызы зор және оны күйдің вириалдық теңдеуімен бағалауға болады. Морзе потенциалы бар екінші вирустық коэффициентті (ВКК) бағалаудың жаңа, практикалық және жалпы аналитикалық әдісі алынды, бұл газдардың барлық термодинамикалық қасиеттерін зерттеу үшін маңызды. Морзе потенциалының аналитикалық формулалары бар SVC бірінші туындысы да анықталған, өйткені ол термодинамикалық өрнектерде кездеседі. Алынған формулалардың мәндерінің бірі олардың параметрлердің барлық диапазондарына қолдану мүмкіндігі болып табылады, бұл дәл және нақты нәтижелерді жылдам қамтамасыз етеді. Қолданған әдістің дәлдігін салыстыру үшін тәжірибелік және аналитикалық деректермен кең диапазоны үшін Ne газының SVC есептеулерімен тексеріледі және He, Ne, Ar, Kr, Xe, H_2, N_2, және O_2 газдардың Бойль температурасы (T_B) жоғары дәлдіктегі сәйкес әдебиет деректері бармен салыстырылады және өзінің құндылығын дәлелденді. Бұл зерттеуде біз сондай-ақ He, Ne, Ar, Kr, Xe, H_2, N_2 және O_2 газдары үшін қысымға байланысты энтропияның, энтальпияның, ішкі энергияның және бос энергияның өзгерістерін алу үшін алынған аналитикалық формулаларын қолдандық. SVC есептеулері үшін газдардың термодинамикалық қасиеттерін алу үшін $(\Delta S)/P$, $\Delta H/P$, $\Delta E/P$ және $\Delta F/P$ нәтижелері ең жиі қолданылатын Ленард-Джонс (12-6) потенциалын пайдаланатын әдебиет деректерімен салыстырылды. Нәтижелер $(\Delta S)/P$ формуласына бұрын еленбеген жоғары ретті терминді қосу дәлдікті жақсартқанын, бірақ шағын үлестерге байланысты әлі де еленбеуге болатынын көрсетті.

Түйін сөздер: Морзе потенциалы, екінші вириалды коэффициент, термодинамикалық қасиеттер.

А.Х. Чачан*, Б.А. Мамедов
Университет Токат Газиосманпаша, г. Токат, Турция
*e-mail: aslihan.cacan@gop.edu.tr

Точная и эффективная теоретическая оценка термодинамических свойств неполярных газов

Исследование межмолекулярных взаимодействий и термодинамических свойств реальных неполярных газов имеет большое значение и может быть оценено с помощью вириального уравнения состояния. В статье получен новый, практичный и общий аналитический метод для оценки второго вириального коэффициента (SVC) с потенциалом Морзе, который важен для исследования всех термодинамических свойств газов. Первая производная SVC с аналитическими формулами потенциала Морзе также установлена, поскольку она появляется в термодинамических выражениях. Одним из значений полученных формул является их применимость для всех диапазонов параметров, что обеспечивает точные результаты быстро. Точность применяемого метода проверена расчетами SVC газа *Ne* для широкого диапазона температур с экспериментальными и аналитическими данными для сравнения и температурой Бойля (T_B) газов *He*, *Ne, Ar, Kr, Xe,* H_2, N_2, и O_2 с включенными высокоточными соответствующими литературными данными для сравнения и доказала свою состоятельность. В этом исследовании также использованы полученные аналитические формулы для получения изменений энтропии, энтальпии, внутренней энергии и свободной энергии в зависимости от давления для газов *He*, *Ne, Ar, Kr, Xe,* H_2, N_2, и O_2. Результаты $\Delta S/P$, $\Delta H/P$, $\Delta E/P$, и $\Delta F/P$ сравниваются с литературными данными, которые используют наиболее часто используемый потенциал Леннарда-Джонса (12-6) для получения термодинамических свойств газов для расчетов SVC. Результаты доказали, что включение ранее игнорированного члена более высокого порядка в формулу $\Delta S/P$ повысило точность, но все еще может быть проигнорировано из-за малых вкладов.

Ключевые слова: потенциал Морзе; второй вириальный коэффициент, термодинамические свойства.

Introduction

Investigation of the interatomic interactions and thermodynamic properties of interacting atoms and molecules depends heavily on the right choice of interaction potential used for virial equation of states via virial coefficients to achieve accurate thermodynamic properties of substances [1-7]. Both Morse and Rydberg potentials provide reliable data for thermodynamic properties, particularly at high temperatures, as their exponential representation of repulsive forces makes them well-suited for generalized chemical models in plasma studies [8]. Although Morse potential displays slightly more attraction than the Rydberg, its relative ease of analytical calculation and good representation of anharmonic oscillator made it commonly used potential in the literature for various fields of research such as DNA denaturation [9], drug design [10], liquid transport properties via molecular dynamics simulation [11], crystal properties of cubic metals [12].

The most reliable Morse potential parameters used in this study were obtained by Matsumoto through analytical calculations with an approximation [13]. Mamedov et al. also established an exact analytical formula for SVC with Morse potential without any approximation but taking its first derivative is a difficult task producing more complicated mathematical formulae to establish related thermodynamic properties [14].

The limitations of applying the Morse potential at low temperatures and the quantum corrections resulting from the high density of materials are discussed in the literature. Although analytical quantum corrections using the Morse potential have been calculated [15], they were not applied in this study because low-temperature conditions were not considered. Analytical solutions, being mathematically expressed, provide a transparent insight into how individual variables and their interplay influence the outcome. Backed with strong statistical theory background by including molecular interactions [16], the analytical solution of Virial Equation of State truncated at the second virial coefficient using Morse potential is used for this study to provide accurate and efficient thermodynamic properties of non-polar gases.

In this study, a simple and practical analytical formula of SVC with Morse potential and its first derivative are established, which is very significant to obtain thermodynamic properties accurately. To our knowledge, this study is the first one in the literature to obtain the simplest analytical solution of SVC with Morse potential and its first derivative and apply them to calculate thermodynamic properties of real systems accurately by comparing the results with the literature using Lennard-Jones (12-6). While Lennard-Jones (12-6) is defined as widely used, two parameter potential for describing van der Waals interactions, Morse potential was designed to represent two body interactions with three parameters making it more convenient for real systems [17].

Methods

Definitions and analytical expressions

The virial equation of state as a power series expansion of number density (ρ) can be expressed as [18]:

$$\frac{P}{R\,T\rho} = Z = 1 + B(T)\rho + C(T)\rho^2 + \cdots, \qquad (1)$$

where Z is the compressibility factor, R is the universal gas constant, $B(T)$ and $C(T)$ are the temperature dependent second and third virial coefficients, respectively.

The second virial coefficient is very important to establish thermodynamic properties and can be given as [19]:

$$B(T) = -2\pi N_A \int_0^\infty \left(e^{-U(r)/k_B T} - 1\right) r^2\, dr \qquad (2)$$

where N_A is the Avogadro's number, k_B is the Boltzmann constant and $U(r)$ is the intermolecular interaction potential which is chosen to be Morse potential in this study in the following form as [20]:

$$U(r) = D_e\left(\left(1 - exp\left(-\beta(r - r_e)\right)\right)^2 - 1\right) \qquad (3)$$

where D_e is the potential well depth which is used in calculations as $D_e/k_B = D_1$ in Kelvins, r_e is the equilibrium distance and β is a parameter determining potentials' curvature at r_e. Eq.(2) becomes Eq.(4) by applying integration by parts to Eq.(2), using Eq.(3) as intermolecular potential:

$$B(T) = -\frac{4\pi N_A D_1}{3T}\left(-\frac{e^{\beta r_e}}{\beta^3}\int_0^1 e^{\frac{2D_1 e^{\beta r_e}u}{T}} e^{\frac{-D_1 e^{2\beta r_e}u^2}{T}} (\ln u)^3\, du + \right.$$
$$\left. + \frac{e^{2\beta r_e}}{\beta^3}\int_0^1 e^{\frac{2D_1 e^{\beta r_e}u}{T}} e^{\frac{-D_1 e^{2\beta r_e}u^2}{T}} u(\ln u)^3\, du \right) \qquad (4)$$

where $u = e^{-\beta r}$. Eq.(4) becomes Eq.(6) after solving the integrations in Eq.(4) and utilizing following series expansion given as [21]:

$$e^{\pm x} = \sum_{i=0}^{\infty} (\pm 1)^i \frac{x^i}{i!} \qquad (5)$$

$$B(T) = -\frac{4\pi N_A D_1}{3T}\sum_{m=0}^{n}\frac{1}{m!}\left(\tfrac{2D_1 e^{\beta r_e}}{T}\right)^m *$$
$$*\left(\frac{3e^{\beta r_e}}{8\beta^3}\Gamma\left(\tfrac{1+m}{2}\right)^4 {}_4\tilde{F}_4\left(\frac{1+m}{2};\frac{3+m}{2};-\tfrac{D_1 e^{2\beta r_e}}{T}\right) - \right. \qquad (6)$$
$$\left. -\frac{6e^{2\beta r_e}}{\beta^3(2+m)^4}\,{}_4F_4\left(1+\frac{m}{2};2+\frac{m}{2};-\tfrac{D_1 e^{2\beta r_e}}{T}\right)\right)$$

The first derivative of the SVC with Morse potential (Eq.(6)) is defined as $B_1(T) = T\frac{dB(T)}{dT}$ and displayed in Eq.(7)

$$B_1(T) = \frac{\pi N_A T}{\beta^3}\left(\sum_{m=0}^{n}\frac{2^{3+m}D_1^{1+m}\left(e^{r_e\beta}\right)^{2+m}}{(2+m)^4\, m!}\left(-\left(1+\frac{m}{2}\right)T^{-2-m}\,{}_3F_3\left(1+\frac{m}{2};2+\frac{m}{2};-\frac{D_1 e^{2r_e\beta}}{T}\right)\right.\right.$$
$$\left. -{}_4F_4\left(1+\frac{m}{2};2+\frac{m}{2};-\frac{D_1 e^{2r_e\beta}}{T}\right) - (1+m)T^{-2-m}\,{}_4F_4\left(1+\frac{m}{2};2+\frac{m}{2};-\frac{D_1 e^{2r_e\beta}}{T}\right)\right)$$
$$-\sum_{m=0}^{n}\frac{2^{-1+m}\left(D_1 e^{r_e\beta}\right)^{1+m}}{m!}\Gamma\left(\frac{1+m}{2}\right)^4\left(\tfrac{(-1-m)}{2}T^{-2-m}\left(\tfrac{1}{\Gamma\left(\frac{3+m}{2}\right)}\,{}_3\tilde{F}_3\left(\frac{1+m}{2};\frac{3+m}{2};-\frac{D_1 e^{2r_e\beta}}{T}\right)\right.\right. \qquad (7)$$
$$\left.\left.\left. -{}_4\tilde{F}_4\left(\frac{1+m}{2};\frac{3+m}{2};-\frac{D_1 e^{2r_e\beta}}{T}\right)\right) - (1+m)T^{-2-m}\,{}_4\tilde{F}_4\left(\frac{1+m}{2};\frac{3+m}{2};-\frac{D_1 e^{2r_e\beta}}{T}\right)\right)\right)$$

where the generalized hypergeometric and regularized generalized hypergeometric functions appearing in Eq.(7) can be defined as, respectively [22]:

$$ {}_pF_q\left(a_1,a_2,...,a_p;b_1,b_2,...,b_q;x\right) = = \sum_{k=0}^{\infty} \frac{\left(a_1\right)_k \left(a_2\right)_k ... \left(a_p\right)_k}{\left(b_1\right)_k \left(b_2\right)_k ... \left(b_q\right)_k} \frac{x^k}{k!}, \quad (8) $$

$$ {}_p\tilde{F}_q\left(a_1,a_2,...,a_p;b_1,b_2,...,b_q;x\right) = = \frac{{}_pF_q\left(a_1,a_2,...,a_p;b_1,b_2,...,b_q;x\right)}{\Gamma\left(b_1\right)...\Gamma\left(b_q\right)} \quad (9) $$

where $\Gamma(z)$ is the gamma function. A simplification of representation demonstrated in Eqs.(10)-(11) is made in Eqs.(6,7) for the generalized hypergeometric and regularized generalized hypergeometric functions since $a_1 = a_2 = \cdots = a_p = a$ and $b_1 = b_2 = \cdots = b_q = b$.

$$ {}_pF_q\left(a;b;x\right) \equiv {}_pF_q\left(a_1,a_2,...,a_p;b_1,b_2,...,b_q;x\right) \quad (10) $$

$$ {}_p\tilde{F}_q\left(a;b;x\right) \equiv \frac{{}_pF_q\left(a;b;x\right)}{\left(\Gamma\left(b\right)\right)^q} \quad (11) $$

Before introducing related thermodynamic functions, a unit conversion of $B(T)$ and $B_1(T)$ is necessary to convert units from cm^3/mol to $cal/mol.atm$ considering that 1 *cal* = 41.293 cm^3.atm. The changes in entropy, enthalpy, internal energy, free energy per pressure in terms of $B(T)$ and $B_1(T)$ can be given as following, respectively [23]:

$$ \frac{\Delta S}{P} = \frac{S - S^0}{P} = -\frac{R\ln P}{P} - \frac{B_1(T)}{T} - \frac{\left(B(T)\right)^2 P}{2RT^2} + ... \quad (12) $$

$$ \frac{\Delta H}{P} = \frac{H - H^0}{P} = B(T) - B_1(T) + ... \quad (13) $$

$$ \frac{\Delta E}{P} = \frac{E - E^0}{P} = -B_1(T) + ... \quad (14) $$

$$ \frac{\Delta F}{P} = \frac{F - F^0}{P} = \frac{RT\ln P}{P} + B(T) + ... \quad (15) $$

Eqs.(12-15) represents the deviations of real gases from their ideal state (the superscript small zero) per pressure at temperature T. The last term in Eq.(12) is neglected in Ref.[17] but included in this study to improve accuracy. Our last calculations include the Boyle temperature at which the SVC value is zero meaning that intermolecular attractions and repulsions are equal and the gas behaves like an ideal one and this temperature value is specific to each gas [24].

Results and Discussion

Table 1 – Morse potential parameters obtained from Ref.[13]

The accuracy of calculated $B(T)$ results of Eq.(6) are compared with the bot experimental and numerical SVC data using Morse potential for Ne at Ref. [25] and confirmed to provide good consistency for the low temperature range of 50-2400 °K as presented at Fig.1(a). For an accurate comparison, Ne potential parameters are considered as $D_1 = 44.6\ °K$, $r_e = 3.0446$ Å and $\beta = 1.85$ Å^{-1} for the Eq.(6) data for the Figure 1(a) as used in Ref.[25]. Another successful data verification of Eq. (6) is displayed in Fig.1(b) for the Ne, by comparing calculated Eq.(6) data with another analytical $B(T)$ data using Morse potential from Ref.[13] which is already calculated in Ref.[14] for the high temperature range of 8000-25000 °K that neutral Ne gas atoms still exist at some proportion depending on temperature value [26]. Morse potential parameters of Ne gas and other gases for the Fig.1(b) is displayed in Table 1.

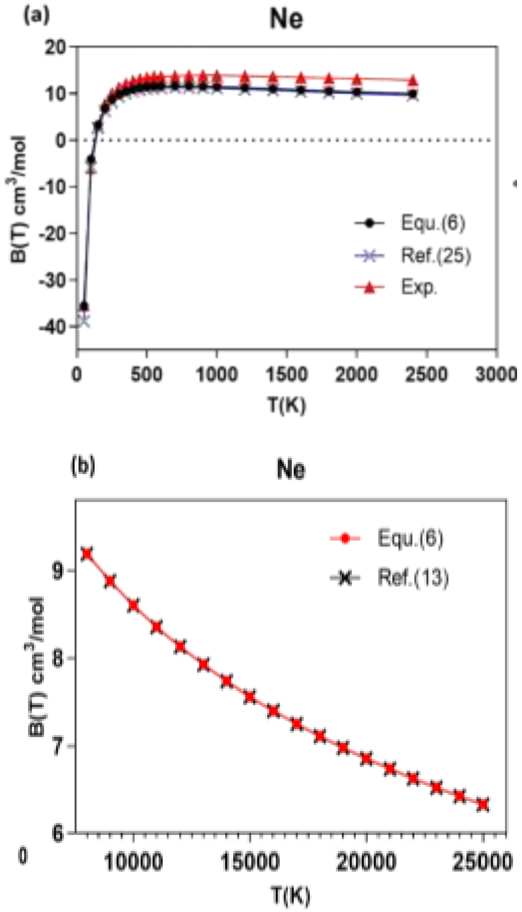


Figure 1 – (a): B(T) values of Ne gas for the low temperature range of 50-2400 $°K$ using Eq.(6), experimental and numerical values from Ref.[25]. (b): B(T) values of Ne gas for the high temperature range of 8000-25000 $°K$ using Eq.(6) and another analytical method using Morse potential at Ref.[13].

	D_1, K	r_e, Å	β, Å^{-1}
He	12.6	2.92	2.197
Ne	51.3	3.09	2.036
Ar	118.1	4.13	1.253
Kr	149.0	4.49	1.105
Xe	226.9	4.73	1.099
H_2	49.4	3.29	1.923
N_2	93.4	4.43	1.166
O_2	152.4	3.75	1.542

The calculated thermodynamic property values of $He, Ne, Ar,\ Kr, H_2, N_2, O_2$ and Xe displayed in Figs. (2-5) are compared with another analytical study using Lennard-Jones (12-6) potential [27] which neglected the higher order term in Eq.(12) for $\Delta S/P$. In general, the calculated values using Morse potential demonstrated good agreement with available literature data using Lennard- Jones (12-6) potential and including the higher order term in Eq.(12) in to the calculations lowered the $\Delta S/P$ values and provided slightly more consistent data with Ref.[27]. It is another fact that, the presence of the higher order term $\left(-(B(T))^2 P/2RT^2\right)$ in calculations slightly improved data reliability but can be neglected since its minor contributions to $\Delta S/P$ for both lower and higher temperature ranges and each graph in Fig.2 includes data without the higher order term in Eq. (12) for the comparison. For instance, the value of $\Delta S/P$ for H_2 at 500 K is $\Delta S/P =$ -0.0000974842 without the higher order term in Eq.(12), however, when the term is included the value is $\Delta S/P =$ -0.000104203.

The same calculation for H_2 is repeated at 5000 K without including the higher order term is $\Delta S/P =$ 0.0000155641, however, when the term is included $\Delta S/P =$ 0.0000155255, both not showing a significant change.

The most noticeable graphs in all figures belongs to Helium since the data of $\Delta S/P$ (Fig. 2), $\Delta H/P$ (Fig.3), and $\Delta E/P$ (Fig. 4) don't display any maximum. A quick analytical evaluation of this work indicated that thermodynamic properties of $\Delta S/P$ and $\Delta H/P$ have a maximum around 400 ⁰K and $\Delta F/P$ has a maximum around 200 ⁰K for the He which is less than our temperature investigation region due to lack of comparable literature data.

Another notable data differences at Fig. 5 become apparent for the $\Delta F/P$ data of He, Ne, H_2, N_2 and O_2 at high temperature region. At the high temperature region, the ΔF/P values diverges more from each other for the Morse and Lennard-Jones (12-6) potentials. The reason for this fact arises from Eq.(15) which displays direct dependency of SVC value (without the unit conversion factor) at the given temperature for a constant pressure value of one atmosphere which is used in this study.

Keeping in mind that the lower SVC data is interpreted as more intermolecular attraction between atom and molecules. Thus, the closer ΔF/P using Morse potential data to negative values as seen in Fig.5 at high temperature region means more dominant intermolecular attraction comparing to data using Lennard-Jones (12-6) potential, which is appropriate for atoms and molecules having tendency for the chemical bonding [1].

Therefore, the obtained thermodynamic properties of gases of H_2, N_2 and O_2 results of this work at high temperature region are more suitable rather than results of noble gases especially for He and Ne. Similarly Fig.5 also displays more positive values for H_2, Ne, Kr and Xe gases at lower temperature region since the closer ΔF/P using Morse potential data to positive values means that intermolecular repulsion is more dominant. This is due to the Morse potential's exponential representation structure of both for the description of intermolecular repulsion and attraction.

Fig. 6 represents the temperature dependence of the changes in entropy, enthalpy, internal energy and free energy per pressure for the Ar gas. The data are calculated by using the Eqs. (12-15) obtained in this work and all of the calculations are completed by using Mathematica 10 programming software.

Table 2 includes the calculated T_B values of different atoms-molecules and compares them with corresponding data of T_B values using artificial neural network (ANN) with hundreds of available experimental SVC data [24, 28] and another data arising from the fitting the equations from National Institute of Standards and Technology (NIST) [29] with low average root-mean-square errors of SVC being 2.94, 3.36 and 3.12 respectively (calculated data only for the relevant gases in table 2 obtained from Ref (24)).

Another analytical results of T_B using SVC with Lennar-Jones (12-6) potential is also included in Table 2 [30]. Our results indicated good consistency with highly accurate literature data.

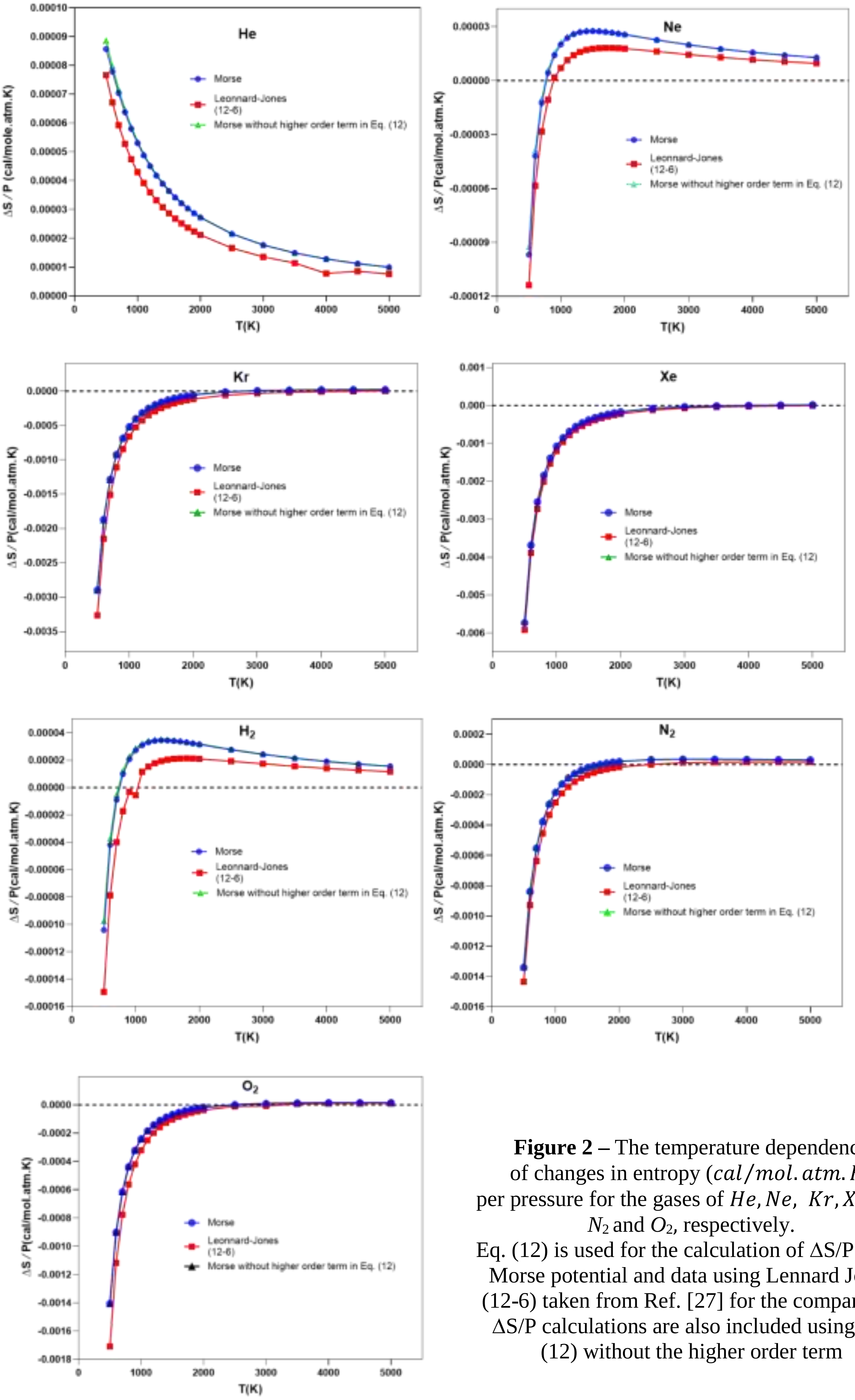


Figure 2 – The temperature dependence of changes in entropy $(cal/mol.atm.K)$ per pressure for the gases of He, Ne, Kr, Xe, H_2, N_2 and O_2, respectively.
Eq. (12) is used for the calculation of ΔS/P using Morse potential and data using Lennard Jones (12-6) taken from Ref. [27] for the comparison. ΔS/P calculations are also included using Eq. (12) without the higher order term

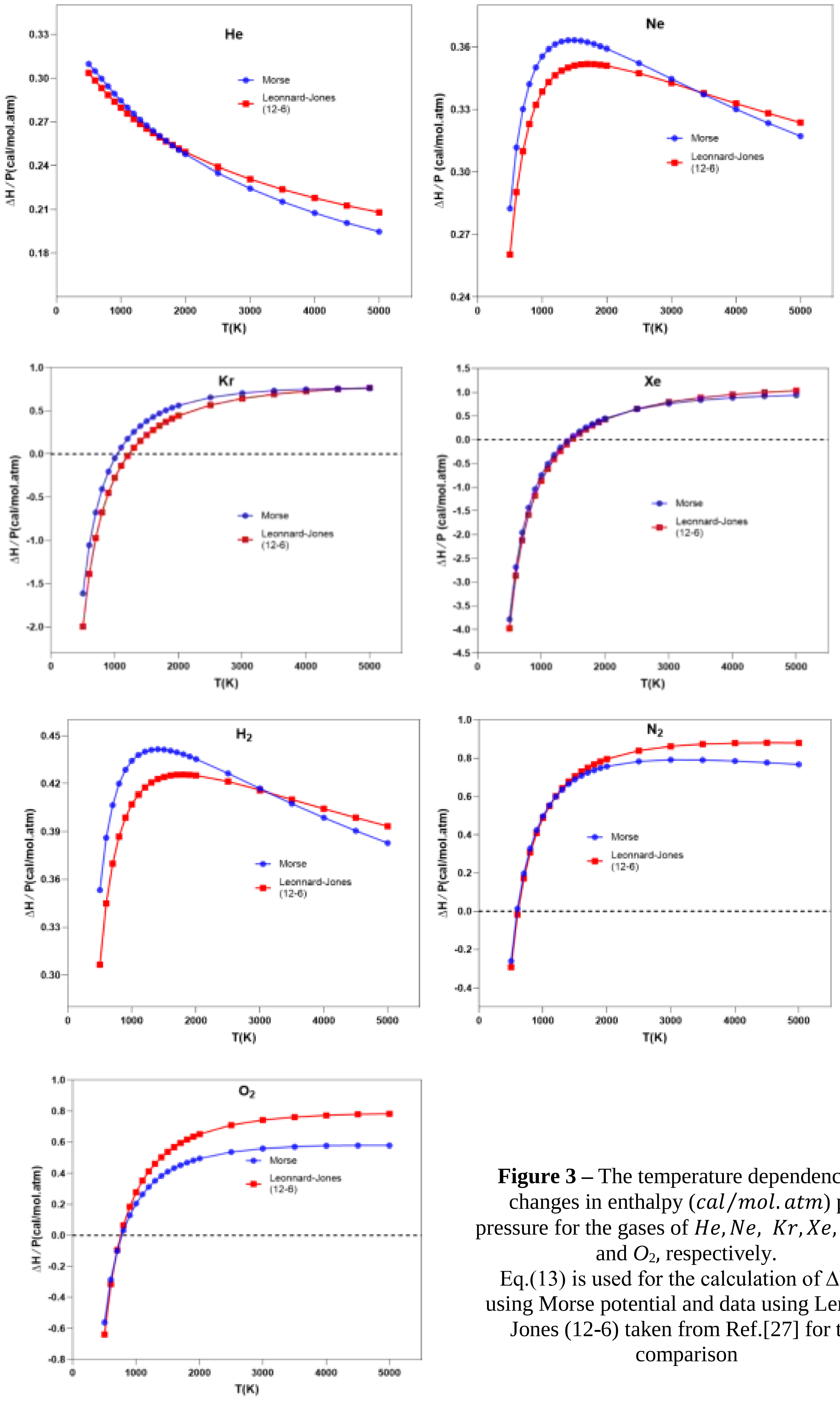
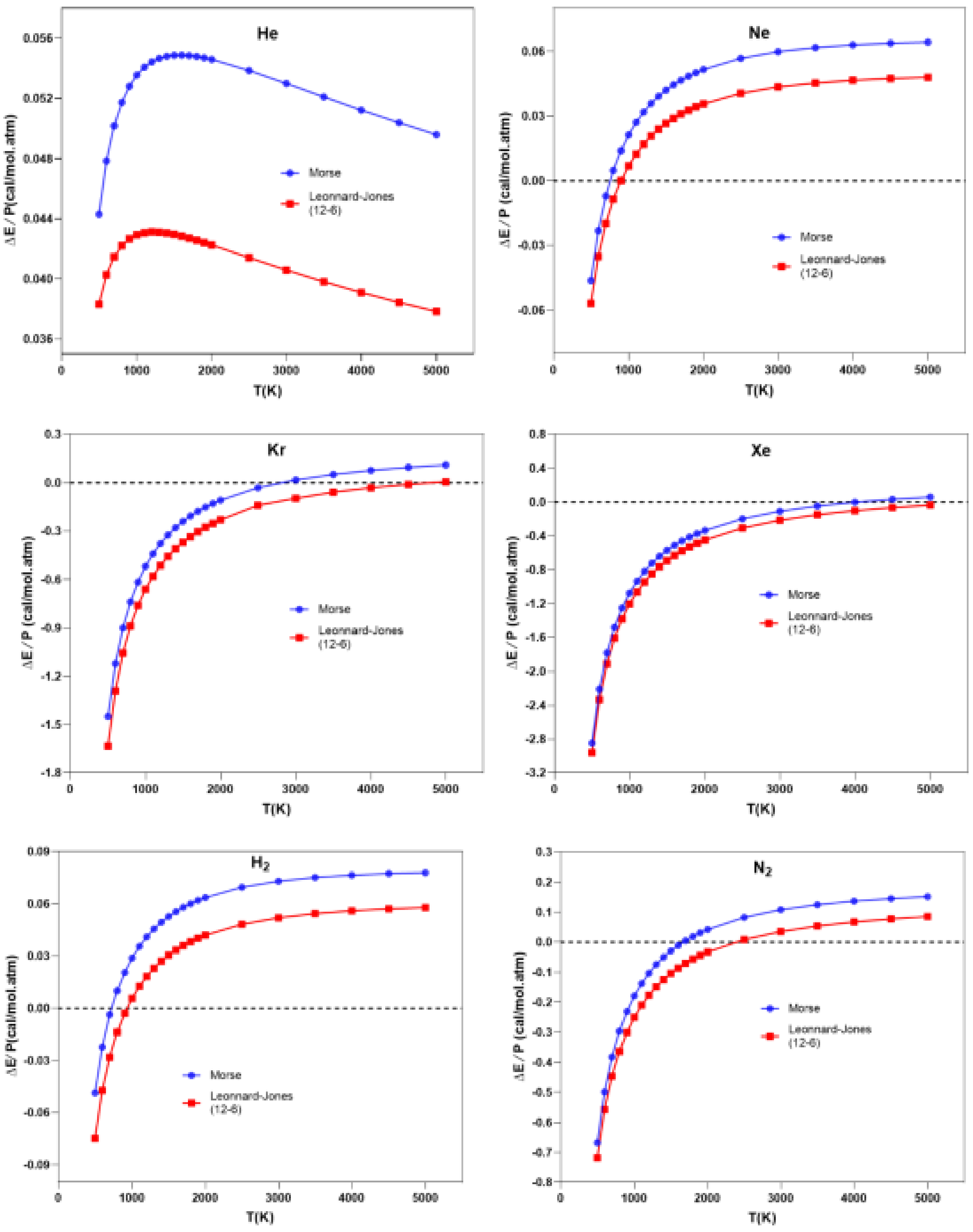


Figure 3 – The temperature dependence of changes in enthalpy ($cal/mol.atm$) per pressure for the gases of $He, Ne,\ Kr, Xe, H_2, N_2$ and O_2, respectively. Eq.(13) is used for the calculation of ΔH/P using Morse potential and data using Lennard Jones (12-6) taken from Ref.[27] for the comparison



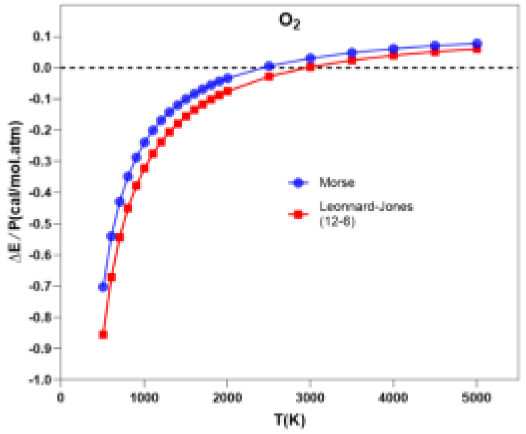


Figure 4 – The temperature dependence of changes in internal energy ($cal/mol.atm$) per pressure for the gases of $He, Ne,\ Kr, Xe, H_2, N_2$ and O_2, respectively.
Eq.(14) is used for the calculation of ΔE/P using Morse potential and data using Lennard Jones (12-6) taken from Ref. (27) for the comparison

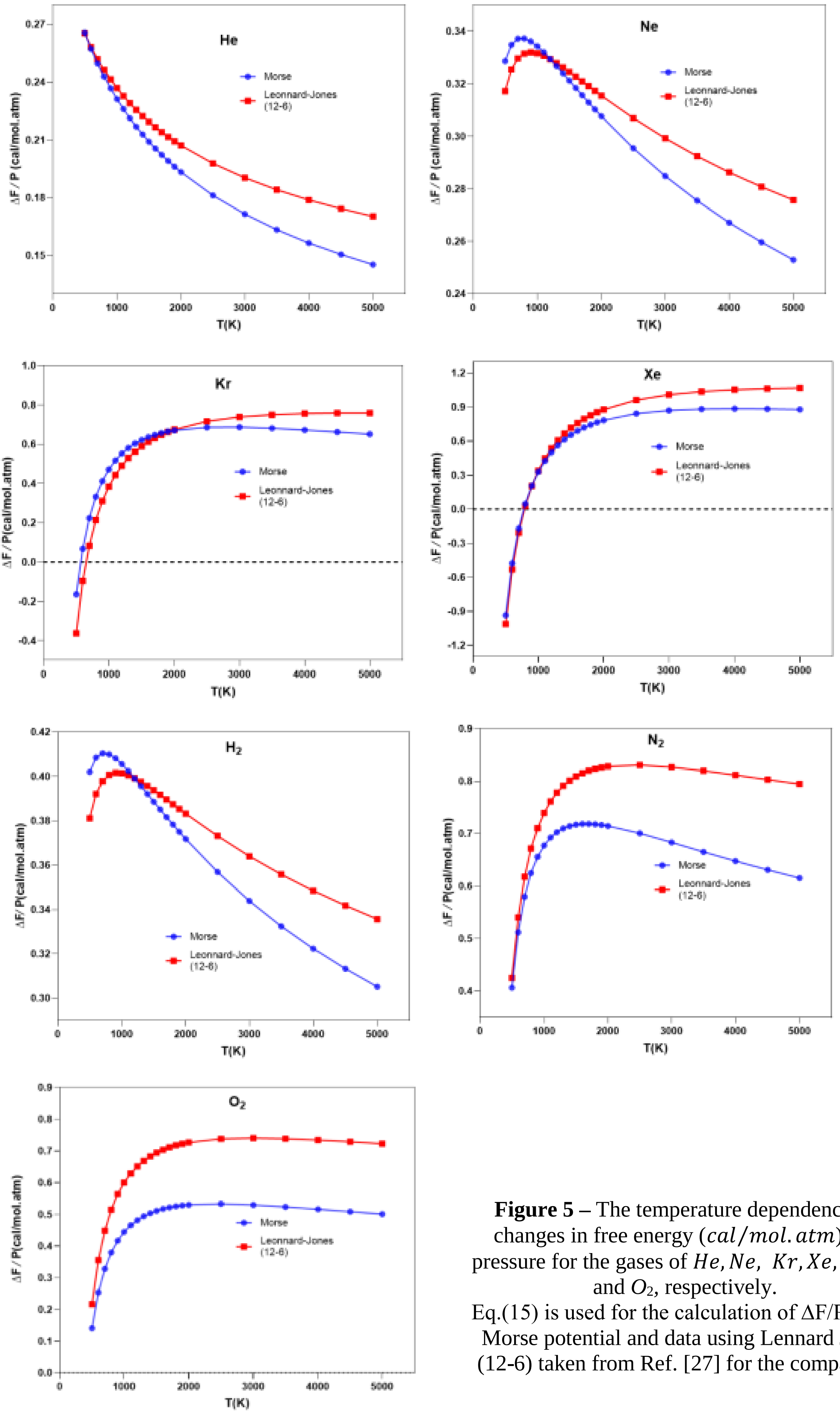


Figure 5 – The temperature dependence of changes in free energy ($cal/mol.atm$) per pressure for the gases of $He, Ne, \ Kr, Xe, H_2, N_2$ and O_2, respectively.
Eq.(15) is used for the calculation of ΔF/P using Morse potential and data using Lennard Jones (12-6) taken from Ref. [27] for the comparison

Table 2- The Calculation of Boyle Temperature of some non-polar atoms and molecules using SVC with Morse potential and corresponding literature data from Refs.[24, 28] being the result of ANN, ata from NIST (Ref.(29)) and Ref.(30) is the analytical one using Lennard-Jones (12-6) potential for the comparison

	T_B this work	Ref. [24]	Ref. [28]	Ref. [29]	T_B from L-J (12-6) Ref [30]
He	28.704	22.86	18.89	23.10	34.93
Ne	120.867	121.97	119.67	119.20	121.678
Ar	407.749	409.06	410.69	411.73	410.151
Kr	566.076	581.92	559.7	600.04	584.466
Xe	775.663	774.97	705.9	773.79	751.944
H_2	115.262	109.73	116.93	109.9	126.463
N_2	323.783	325.6	345.5	327.01	N/A
O_2	418.875	401.19	413.57	404.47	403.316

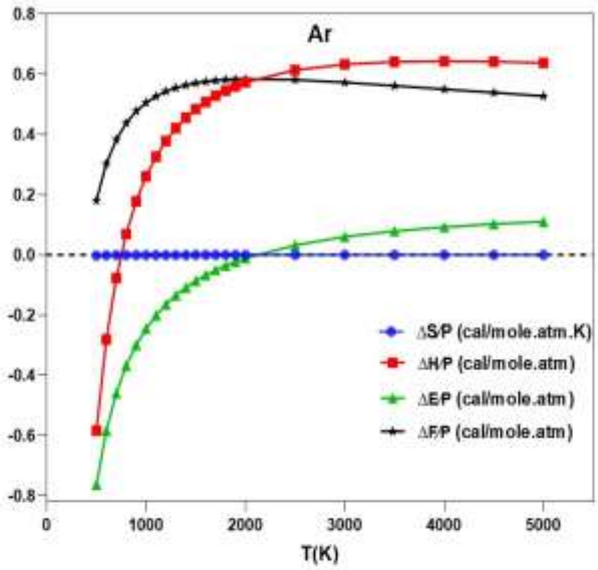


Figure 6 – The temperature dependence of changes in entropy, enthalpy, internal energy and free energy per pressure for the Ar gas. The calculations were made based on the Eqs. (12-15).

Conclusion

Analytical $B(T)$ calculations are proved to be consistent with literature both for high and low temperature ranges. The accuracy is also proved by the calculations of T_B with this analytical method using SVC with Morse potential and the results are compared with the highly accurate T_B calculations using ANN with numerous available experimental data of SVC from literature. The thermodynamic results of $\Delta S/P$, $\Delta H/P$, $\Delta E/P$, and $\Delta F/P$ for the He, Ne, Ar, Kr, Xe, H_2, N_2 and O_2 gases are also compared with the literature data using Lennard-Jones (12-6) potential for SVC calculations [27] and found to be slightly improved for the entropy values. In this study, this term is included in calculations leading to slightly more accurate and precise data with simple analytical formulae. The calculated results indicated good consistency with both for experimental and analytical literature data and provided reliable thermodynamic properties without any parameter restrictions and experimental data limitations by using Morse potential for the SVC and its first derivative in analytical thermodynamic calculations for the first time in literature. Further investigations will be made to achieve second derivative of SVC to obtain more thermodynamic properties.

References

1 Kaplan I.G. Intermolecular Interactions: Physical Picture, Computational Methods and Model Potentials. – Jonh Wiley & Sons, 2006. – P.146-150.

2 Sadus R. J. Two-body Intermolecular Potentials from Second Virial Coefficient Properties // J.Chem.Phys. – 2019. – Vol.150. – Art. 024503.

3 González-Calderón A., Rocha-Ichante, A. Second Virial Coefficient of a Generalized Lennard-Jones Potential. //J.Chem.Phys. – 2015. – Vol.142. – Art. 034305.

4 Bai J., Zhang P., Zhou, C-W., Zhao H. Theoretical studies of real-fluid oxidation of hydrogen under supercritical conditions by using the virial equation of state // Combust. Flame. – 2022. – Vol. 241. – Art.112060

5 Kwon T, Song H.W., Woo S.Y., Kim J.-H., Sung,Bull B.J. The accurate estimation of the third virial coefficients for helium using three-body neural network potentials. // Korean Chem. Soc. – 2022. – Vol.43(5). – P.612.

6 Zeng X.L., Ju X.H., Xu S.Y. Interatomic Potential and Thermodynamic Property of Diatomic Uranium. // Adv. Mat. Res. – 2012. – Vol.550-553. – P.2810-2813.

7 Mamedov B.A., Somuncu E., Askerov I.M., Evaluation of Speed of Sound and Specific Heat Capacities of Real Gases. // J. Thermophys. Heat. Tr. – 2018. – Vol.32. – P.984-998.

8 Apfelbaum E.M. Calculation of Thermophysical Properties of Titanium and Zinc Plasmas // High. Temp. – 2017. – Vol.55. – P.1-11.

9 Kinani R., Kaidi H., Benhamou M. Investigation of DNA Denaturation from Generalized Morse Potential. // Mater. Devices. – 2018. – Vol. 3. – P.0207.

10 Monajjemi M., Naderi F., Mollaamin F., Khaleghian M. Drug Design Outlook by Calculation of Second Virial Coefficient as a Nano Study. // J. Mex. Chem. Soc. – 2012. – Vol.56. – P.207-211.

11 Galicia-Pimentel U.F., Osorio-Gonz´alez D., L´opez-Lemus J. On the Morse Potential in Liquid Phase and at Liquid-Vapor Interface. // Rev. Mex. Fis. – 2006. – Vol.52. – P.422-428.

12 Pirog I.V., Nedoseikina T.I. Study of Effective Pair Potentials in Cubic Metals // Physica B Condens. Matter. – 2003. – Vol.334. – P.123-129.

13 Matsumoto A. Parameters of the Morse Potential from Second Virial Coefficients of Gases. // Zeitschrift für Naturforschung A. – 1987. – Vol.42a. – P.447-450.

14 Mamedov B.A., Cacan H. A general analytical method for evaluation of the thermodynamic properties of matters using virial coefficients with Morse potential at high temperature. // Contrib. Plasm. Phys. – 2019. – Vol. 59. – Art.e201900021.

15 Cacan H., Mamedov B. A. The Comparative Analytical Evaluation of Quantum Corrections to the Second Virial Coefficient with Morse Potential and its Applications to Real Systems. // J. Chem. Thermodyn. 2019,138, 147-150.

16 Hall K.R., and Iglesias-Silva G.A. Generalized Derivations for Mixtures Using The Virial Equation: Application to Fugacity. // Chem. Eng. Commun. – 1995. – Vol.137(1). – P.211–214. DOI: 10.1080/00986449508936377

17 Lim T. The Relationship between Lennard-Jones (12-6) and Morse Potential Functions. // Z. Naturforsch A. – 2003. – Vol.58(11). – P.615-617. DOI: 10.1515/zna-2003-1104

18 Harvey A.H., Lemmon E.W. Correlation for the Second Virial Coefficient of Water. // Journal of Physical and Chemical Reference Data. – 2004. – Vol.33(1). – P.369–376.

19 Sadus R.J. Second Virial Coefficient Properties of the n-m Lennard-Jones/Mie Potential. // J.Chem.Phys. – 2018. – Vol.149. – Art. 074504.

20 Nickabadi S., Ansari R., Rouhi S. Evaluation of the Morse Potential Function Coefficients for Germanene by the First Principles Approach. // J Mol Graph Model. – 2020. – Vol.98. – Art. 107589.

21 Gradshteyn I.S., Ryzhik I.M. Table of Integrals, Series and Products. – Acedemic Press, London Acedemic Press, 2014. – P.25-62.

22 Abramowitz M., Stegun I. Handbook of Mathematical Functions. – Dover Publications, Inc., 1974. – P.555-567.

23 O'Connell J.P., Haile J.M. Thermodynamics: Fundamentals for Applications. – Cambridge University Press, 2005. – P.155-180.

24 Coccia G., Di Nicola G. Determination of the Boyle temperature of pure gases using artificial neural network. // Fluid Phase Equilibria. – 2019. – Vol.493. – P.36-42.

25 Al-Maaitah A.F. A Microscopic Study of Ne-Ne Interactions with Phenomenological Potentials Using Second Virial Coefficients. // Sci.Int. (Lahore). – 2020. – Vol.32(1). – P.1-6.

26 Ebeling W., Fortov V.E., Filinov V. Quantum Statistics of Dense Gases and Nonideal Plasmas. – Springer, Cham 2017.

27 Mamedov B.A., Somuncu E. Accurate Evaluation of the Internal Energy, Free Energy, Entropy and Enthalpy of Non-Polar Molecules by using Virial Coefficients. // Chin. J. Phys. – 2017. – Vol.55. – P.1473-1488.

28 Di Nicola G., Coccia G., Pierantozzi M., Tomassetti S., Grifoni R.C. Artificial neural network for the second virial coefficient of organic and inorganic compounds: An ANN for B of organic and inorganic compounds // Chemical Engineering Communications. – 2018. – Vol.205(8). – P.1077-1095.

29 Dymond J., Marsh K., Wilhoit R., Wong K. Virial Coefficients of Pure Gases, Landolt-Bornstein: Numerical Data and Functional Relationships in Science and Technology. –Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology, 2005.

30 Somuncu E. Accurate assessment of the Boyle temperature of nonpolar molecular gases using second virial coefficient with Lennard-Jones (12-6) potential // Indian J Phys. – 2019. – Vol.93. – P.565–569.

References

1 I. G. Kaplan, Intermolecular Interactions: Physical Picture, Computational Methods and Model Potentials (Jonh Wiley & Sons, 2006), pp. 146–150.

2 R.J. Sadus, J. Chem. Phys. 150, Art. 024503 (2019). DOI: 10.1063/1.5067267.

3 A. González-Calderón and A. Rocha-Ichante, J. Chem. Phys. 142, 034305 (2015). DOI: 10.1063/1.4905548.

4 J. Bai, P. Zhang, C.-W. Zhou, and H. Zhao, Combust. Flame 241, 112060 (2022). DOI: 10.1016/j.combustflame.2022.112060.

5 T. Kwon, H.W. Song, S.Y. Woo, and J.-H. Kim, Bull. Korean Chem. Soc. 43, 612 (2022). DOI: 10.1002/bkcs.12358.

6 X.L. Zeng, X.H. Ju, and S.Y. Xu, Adv. Mater. Res. 550–553, 2810–2813 (2012). DOI: 10.4028/www.scientific.net/AMR.550-553.2810.

7 B.A. Mamedov, E. Somuncu, and I.M. Askerov, J. Thermophys. Heat Transf. 32, 984–998 (2018). DOI: 10.2514/1.T5417.

8 E.M. Apfelbaum, High Temp. 55, 1–11 (2017). DOI: 10.1134/S0018151X17010013.

9 R. Kinani, H. Kaidi, and M. Benhamou, Mater. Devices 3, 0207 (2018).

10 M. Monajjemi, F. Naderi, F. Mollaamin, and M. Khaleghian, J. Mex. Chem. Soc. 56, 207–211 (2012). DOI: недоступен.

11 U.F. Galicia-Pimentel, D. Osorio-González, and J. López-Lemus, Rev. Mex. Fis. 52, 422–428 (2006). DOI: недоступен.

12 I.V. Pirog and T.I. Nedoseikina, Physica B Condens. Matter 334, 123–129 (2003). DOI: недоступен.

13 A. Matsumoto, Z. Naturforsch. A 42a, 447–450 (1987). DOI: недоступен.

14 B.A. Mamedov and H. Cacan, Contrib. Plasma Phys. 59, e201900021 (2019). DOI: 10.1002/ctpp.201900021.

15 H. Cacan and B.A. Mamedov, J. Chem. Thermodyn. 138, 147–150 (2019). DOI: 10.1016/j.jct.2019.07.015.

16 K.R. Hall and G.A. Iglesias-Silva, Chem. Eng. Commun. 137, 211–214 (1995). DOI: 10.1080/00986449508936377.

17 T. Lim, Z. Naturforsch. A 58, 615–617 (2003). DOI: 10.1515/zna-2003-1104.

18 A.H. Harvey and E.W. Lemmon, J. Phys. Chem. Ref. Data 33, 369–376 (2004). DOI: 10.1063/1.1649348.

19 R.J. Sadus, J. Chem. Phys. 149, 074504 (2018). DOI: 10.1063/1.5044669.

20 S. Nickabadi, R. Ansari, and S. Rouhi, J. Mol. Graph. Model. 98, 107589 (2020). DOI: 10.1016/j.jmgm.2020.107589.

21 I.S. Gradshteyn and I.M. Ryzhik, Table of Integrals, Series and Products (Academic Press, 2014), pp. 25–62.

22 M. Abramowitz and I. Stegun, Handbook of Mathematical Functions (Dover Publications, Inc., 1974), pp. 555–567.

23 J. P. O’Connell and J. M. Haile, Thermodynamics: Fundamentals for Applications (Cambridge University Press, 2005), pp. 155–180.

24 G. Coccia and G. Di Nicola, Fluid Phase Equilib. 493, 36–42 (2019). DOI: 10.1016/j.fluid.2019.03.017.

25 A.F. Al-Maaitah, Sci. Int. (Lahore) 32, 1–6 (2020).

26 W. Ebeling, V. E. Fortov, and V. Filinov, Quantum Statistics of Dense Gases and Nonideal Plasmas (Springer, Cham, 2017).

27 B.A. Mamedov and E. Somuncu, Chin. J. Phys. 55, 1473–1488 (2017). DOI: 10.1016/j.cjph.2017.07.011.

28 G. Di Nicola, G. Coccia, M. Pierantozzi, S. Tomassetti, and R. C. Grifoni, Chem. Eng. Commun. 205, 1077–1095 (2018). DOI: 10.1080/00986445.2018.1432051.

29 J. Dymond, K. Marsh, R. Wilhoit, and K. Wong, Virial Coefficients of Pure Gases (Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology, 2005).

30 E. Somuncu, Indian J. Phys. 93, 565–569 (2019). DOI: 10.1007/s12648-018-01356-6.

Article history:
Received 30 October 2024
Accepted 18 December 2024

Information about authors:

1. **Aslihan Hatun Cacan** (corresponding author) – Tokat Gaziosmanpasa University, Faculty of Engineering and Natural Sciences, Tokat, Turkey; e-mail: aslihan.cacan@gop.edu.tr

2. **Bahtiyar Mamedov –** Tokat Gaziosmanpasa University, Department of Physics, Tasliciftlik Campus, Tokat, Turkey; e-mail: bamamedov@yahoo.com

Мақала тарихы:
Түсті – 30.10.2024
Қабылданды – 18.12.2024

Авторлар туралы мәлімет:

1. **Аслыхан Хатун Чачан** (автор-корреспондент) – Токат Газиосманпаша университеті, инженерлік және ғылым факультеті, Токат қ., Түркия; e-mail: aslihan.cacan@gop.edu.tr

2. Бақтияр Мамедов – Токат Газиосманпаша университеті, физика факультеті, Тасличифтлик кампусы, Токат қ., Түркия; e-mail: bamamedov@yahoo.com