Unified Analytical Formulae of Second Virial Coefficient with Kihara Potential and its Application to Real Gases

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We propose a general evaluation method to calculate the second virial coefficient with Kihara potential (spherical core). The suggested approach is based on exponential function series expansion formula and gamma functions, which enable us to have accurate evaluation of the second virial coefficient. The results of second virial coefficient determined from Kihara potential are compared with the calculations of second virial coefficient with Lennard–Jones (12-6) potential. The analytical formula allows an accurate determination of Boyle temperature of gases. The accuracy of the obtained formula is tested by its application to gases Ar, Kr, Ne, CH_4, C_6H_6, C_3H_8, n-C_4H_{10}, and n-C_5H_{12}. The results of the second virial coefficient in a wide temperature range and Boyle temperature are in good agreement with the data available in the literature.

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1. Introduction

The evaluation of the virial coefficients is an important issue to determine intermolecular interactions with arbitrary values of temperature and thermodynamic properties of real gases [1–8]. In literature, several experimental and theoretical methods have been proposed to obtain accurate and efficient evaluation of the second virial coefficient with various types of potentials [9–16]. The Lennard–Jones ($2n$-n) potential that is important to define the interaction between simple spherical molecules only, has been widely studied by both experimental and theoretical methods [17]. Kihara potential is defined of the interaction between two more complex molecules and found wide applications because it is superior to Lennard–Jones (12-6) potential for determination of virial coefficients, thermodynamic and transport properties [18–20]. There are also some restricted studies on the analytical evaluation of second virial coefficient with Kihara potential [20–22]. In spite of many studies, the applications of the second virial coefficient for various types of the intermolecular interaction are still one of the main actual problems in physics and biophysical chemistry [23–25].

In this paper, an efficient analytical formula for the second virial coefficient with Kihara potential is presented. For some of gases, examples of applications are given to demonstrate the efficiency of the present analytical expression. For gases Ar, Kr, Ne, CH_4, C_6H_6, C_3H_8, n-C_4H_{10}, and n-C_5H_{12}, we have calculated the Boyle temperature by using obtained formula. The calculation results for the second virial coefficient with Kihara potential and its implementation to the various gases indicate a good rate of convergence and numerical stability.

2. Expressions for the Second Virial Coefficient with Kihara Potential and Boyle Temperature

The second virial coefficient in terms of intermolecular potential $u(r_{ij})$ are given in the following forms [21]

$$B_2(T) = -2\pi N_{\mathrm{A}} \int_0^{\infty} r_{12}^2 \left(\mathrm{e}^{-u(r_{12})/k_{\mathrm{B}}T} - 1\right) \mathrm{d}r_{12} \tag{1}$$

where N_{A} is Avogadro's constant, k_{B} is the Boltzmann constant and T is temperature. The physical significance of second virial coefficient is that it demonstrates the first deviation from ideality [21, 26, 27]. The temperature at which $B_2(T) = 0$ is called the Boyle temperature [27]. At Boyle temperature, the gases appear to behave ideally.

For evaluation of the second virial coefficient, we use the Kihara potential for molecules with spherical cores of the following form [22]:

$$u(r) = \begin{cases} \infty & r < d \\ 4\varepsilon \left[\left(\frac{\sigma-d}{r-d}\right)^{12} - \left(\frac{\sigma-d}{r-d}\right)^{6}\right] & r \geq d \end{cases} \tag{2}$$

where d is the radius of spherical molecular core, ε is the depth of the potential well, σ is the collision diameter, and r is the distance between the particles [28]. Equation (2) gives the Lennard–Jones (12-6) potential, when $d = 0$ [28].

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Inserting (2) into (1) leads to

$$B_2(T^*) = -2\pi N_{\mathrm{A}}\left(\frac{\sigma}{1+a^*}\right)^3\left\{-\int\limits_0^{a^*} x^2\,\mathrm{d}x + \int\limits_{a^*}^{\infty}\left[\exp\left(-\frac{4}{T^*}\left((x-a^*)^{-12}-(x-a^*)^{-6}\right)\right)-1\right]x^2\,\mathrm{d}x\right\}, \tag{3}$$

where $T^* = k_{\mathrm{B}}T/\varepsilon$, $r/\sigma - d = x$, $d/\sigma - d = a^*$, and $d = a^*\sigma/(1+a^*)$. By applying partial integral to the second term in (3), we obtain the following formula:

$$B_2(T^*) = -2\pi N_{\mathrm{A}}\left(\frac{\sigma}{1+a^*}\right)^3\frac{4}{3T^*}$$
$$\times\int\limits_{a^*}^{\infty}\exp\left(-\frac{4}{T^*}\left((x-a^*)^{-12}-(x-a^*)^{-6}\right)\right)\left(-12\,(x-a^*)^{-13}+6\,(x-a^*)^{-7}\right)x^3\,\mathrm{d}x. \tag{4}$$

To evaluate integrals we use a well-known series formula of exponential functions as [29]

$$e^{\pm x} = \sum_{n=0}^{N}(\pm 1)^n\frac{x^n}{n!}. \tag{5}$$

By subsisting (5) into (4), we have

$$B_2(T^*) = 2\pi N_{\mathrm{A}}\left(\frac{\sigma}{1+a^*}\right)^3$$
$$\times\left[\frac{8}{T^*}\lim_{N=\to\infty}\sum_{n=0}^{N}\frac{(4/T^*)^n}{n!}\int\limits_{a^*}^{\infty}\exp\left(-\frac{4\,(x-a^*)^{-12}}{T^*}\right)(x-a^*)^{-6n}\left(2\,(x-a^*)^{-13}-(x-a^*)^{-7}\right)x^3\,\mathrm{d}x\right]. \tag{6}$$

Further, solving integral in (6) allows to obtain

$$B_2(T^*) = \frac{8\pi N_{\mathrm{A}}}{3T^*}\lim_{N=\to\infty}\sum_{n=0}^{N}\frac{(4T^*)^n}{n!}$$
$$\times(\sigma-d)^{12+6n}\left[d^3\left(\frac{4/T^*}{(\sigma-d)^{-12}}\right)^{-\left(\frac{n}{2}+1\right)}\Gamma\left(\frac{n}{2}+1\right)+3d^2\left(\frac{4/T^*}{(\sigma-d)^{-12}}\right)^{-\left(\frac{n}{2}+\frac{11}{12}\right)}\Gamma\left(\frac{n}{2}+\frac{11}{12}\right)\right.$$
$$\left.+3d\left(\frac{4/T^*}{(\sigma-d)^{-12}}\right)^{-\left(\frac{n}{2}+\frac{5}{6}\right)}\Gamma\left(\frac{n}{2}+\frac{5}{6}\right)+\left(\frac{4/T^*}{(\sigma-d)^{-12}}\right)^{-\left(\frac{n}{2}+\frac{3}{4}\right)}\Gamma\left(\frac{n}{2}+\frac{3}{4}\right)\right]$$
$$-\frac{1}{2}(\sigma-d)^{-6}\left[d^3\left(\frac{4/T^*}{(\sigma-d)^{-12}}\right)^{-\left(\frac{n}{2}+\frac{1}{2}\right)}\Gamma\left(\frac{n}{2}+\frac{1}{2}\right)+3d^2\left(\frac{4/T^*}{(\sigma-d)^{-12}}\right)^{-\left(\frac{n}{2}+\frac{5}{12}\right)}\Gamma\left(\frac{n}{2}+\frac{5}{12}\right)\right.$$
$$\left.+3d\left(\frac{4/T^*}{(\sigma-d)^{-12}}\right)^{-\left(\frac{n}{2}+\frac{1}{3}\right)}\Gamma\left(\frac{n}{2}+\frac{1}{3}\right)+\left(\frac{4/T^*}{(\sigma-d)^{-12}}\right)^{-\left(\frac{n}{2}+\frac{1}{4}\right)}\Gamma\left(\frac{n}{2}+\frac{1}{4}\right)\right] \tag{7}$$

With the use of function

$$H(u,k) = \lim_{N\to\infty}\sum_{t=0}^{N}(4/T^*)^t\left(\frac{\sigma}{1+a^*}\right)^{12+6t}u^{-\frac{6t+k}{12}}\Gamma\left(\frac{6t+k}{12}\right) \tag{8}$$

simpler form of (7) can be obtained, namely:

$$B_2(T^*) = \frac{8\pi N_{\mathrm{A}}}{3T^*} \tag{9}$$
$$\times\left\{d^3H\left(\frac{4/T^*}{(\sigma-d)^{-12}},12\right)+3d^2H\left(\frac{4/T^*}{(\sigma-d)^{-12}},11\right)+3dH\left(\frac{4/T^*}{(\sigma-d)^{-12}},10\right)+H\left(\frac{4/T^*}{(\sigma-d)^{-12}},9\right)\right.$$
$$\left.-\frac{1}{2}(\sigma-d)^{-6}\left[d^3H\left(\frac{4/T^*}{(\sigma-d)^{-12}},6\right)+d^2H\left(\frac{4/T^*}{(\sigma-d)^{-12}},5\right)+3dH\left(\frac{4/T^*}{(\sigma-d)^{-12}},4\right)+H\left(\frac{4/T^*}{(\sigma-d)^{-12}},3\right)\right]\right\}$$

where N is the upper limits of summation. The reduced second virial coefficient is $B_2^*(T^*) = B_2(T^*)/b_0$, where $b_0 = \frac{2\pi}{3} N_A \sigma^3$. The quantity $\Gamma(\alpha)$ is well known gamma function defined by [29]

$$\Gamma(\alpha) = \int_0^\infty e^{-t} t^{\alpha-1} \, dt \tag{10}$$

In this paper, we calculate the Boyle temperature T_B by using the following condition in (9):

$$B_2(T_B^*) = 0 \tag{11}$$

4. Numerical results and discussion

In this work, the second virial coefficient with Kihara potential has been studied with the analytical evaluations. The Mathematica 7.0 international software has been used to calculate the analytical expression. The second virial coefficients with Kihara potential and Lennard–Jones (12-6) potential have been plotted and the influence of parameters values on the results have been analyzed. The results show that the obtained expression is general and valid for arbitrary values of parameters. The calculated results are compared with the corresponding experimental and other theoretical values [20, 22, 30]. The accuracy of analytical method is satisfactory and can be suggested for evaluation of thermodynamic properties of gases by using second virial coefficient.

A theoretical method based on the gamma function was used for the evaluation of second virial coefficient with Kihara potential in [5, 20, 31]. The difference between [5, 20, 31] and the results in this paper is caused by the analytical calculation method. To show the effectiveness of the proposed method we apply it for molecules Ar, Kr, Ne, CH_4, C_6H_6, C_3H_8, n-C_4H_{10}, and n-C_5H_{12}. In Tables I–III, the accuracy of the analytical formula is demonstrated by comparison of different results from experimental data, theoretical data [5, 20, 31], and Lennard–Jones (12-6) potential results [15, 21]. As can be seen from Table II, the obtained results for the second virial coefficient of Kihara potential by using different parameter values are in better agreement with experimental data than [20] and/or the calculated results of the second virial coefficient with Lennard–Jones (12-6) potential.

As it is demonstrated in Table IV, the convergence properties of (9) with those in [20] change wildly. The most rapid convergence to the numerical results for different values of T^* shows (9). The calculations have been made with the upper limits $N = 50$ series.

The examples of calculations of (9) for gases Ar, Kr, Ne, CH_4, C_6H_6, C_3H_8, n-C_4H_{10}, and n-C_5H_{12} are presented in Tables I–III and Figs. 1, 2. It is understood from the resolution of the graphics that the results are in good agreement with data available in literature [27–29]. For a wide range of temperature the results of (9) show agreement with the literature [20, 22, 32]. However, for increased values of a^* there is less agreement. Examples for $a^* = 0$ (Lennard–Jones limit) are given in Table I. The results of the calculation according to Eq. (9) agrees with those in [15, 21]. In Figs. 1, 2 we compare our studies with results from [22, 30] and the agreements are satisfactory. Also, the results of second virial coefficient for Kihara potential show a good agreement with calculated results of second virial coefficients determined from Lennard–Jones (12-6) potential [32]. The reduced Boyle's temperature, obtained by us using the second virial coefficient, is $T_B^* = 2.8771$ [33]. At this temperature real gas is considered as an ideal gas.

The parameters of Lennard–Jones (12-6) potential [15, 34] and Kihara potential [22, 28] are represented in Table V for gases Ar, Kr, Ne, CH_4, C_6H_6, C_3H_8, n-C_4H_{10} and n-C_5H_{12}. These gases are used widely in industry, and in scientific and engineering applications, thus the analytical expression provides the access to exact calculation of second virial coefficient with Kihara potential. The obtained results for the second virial coefficient by using different parameter values of Kihara potential are shown in Table II. The presented values are very close to each other. As can be seen from Table II, the calculated second virial coefficient as a function of temperature when compared with experimental values show very good agreement. In fact, this agreement is even better than for those using the Lennard–Jones (12-6) potentials.

To sum up, further academic backgrounds and further discussion of their results are required. The main contribution of this work is the addition of new relationships of the well-known second virial coefficient of Kihara potential with spherical core. In addition, the accuracy of computation is analyzed and a theoretical assessment of virial to real gases has been performed.

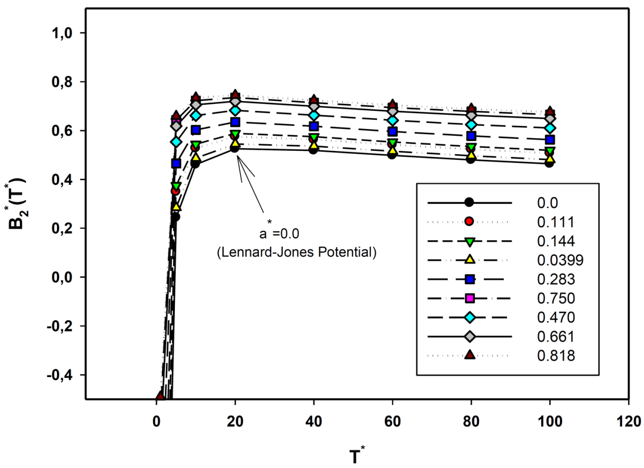

Fig. 1. The reduced temperature dependence of reduced second virial coefficients various a^* of potential parameter.

TABLE I

Calculation results of second virial coefficient $B_2^*(T^*)$ with Kihara potential.

a^*	T^*									
	0.000	0.000[a]	0.111	0.144	0.0399	0.283	0.750	0.470	0.661	0.818
0.50	−8.72021	−8.72021	−7.30713	−6.95861	−8.16383	−5.75048	−3.42537	−4.58775	−3.74069	−3.21053
0.80	−3.73423	−3.73423	−3.02712	−2.85337	−3.45533	−2.25334	−1.11018	−1.67955	−1.26417	−1.00547
1.00	−2.53808	−2.53808	−2.00609	−1.8755	−2.32816	−1.42494	−0.568734	−0.994782	−0.683876	−0.490484
5.00	0.243344	0.243344	0.348585	0.374637	0.284714	0.465317	0.642146	0.553278	0.617927	0.6587
10.0	0.460875	0.460875	0.527116	0.543767	0.486729	0.602633	0.722444	0.661289	0.705566	0.734081
20.0	0.525374	0.525374	0.575458	0.588313	0.544729	0.634693	0.734234	0.682496	0.719749	0.744318
40.0	0.518575	0.518575	0.562969	0.574595	0.535563	0.617351	0.713523	0.662774	0.699147	0.723607
60.0	0.498213	0.498213	0.541629	0.553113	0.514745	0.595737	0.693742	0.641672	0.678914	0.70418
80.0	0.47979	0.47979	0.523072	0.534591	0.49622	0.577591	0.677795	0.624337	0.662523	0.688565
100	0.464069	0.464069	0.507445	0.519039	0.480498	0.562496	0.664719	0.610029	0.649061	0.675777

[a]Ref. [15, 21]

TABLE II

Comparison of the results obtained from Equation (9), different parameter values of Kihara potential [5, 22, 28], Lennard–Jones (12-6) potential and experimental data for Ar, Kr and Ne.

$T\,(K)$	Eq. (9)	Kihara Potential			Lennard–Jones (12-6) Potential [15, 21]	Experimental data [22, 30]
		Ref. [28]	Ref. [5]	Ref. [20]		
Ar						
105.50	−165.942	−165.233	−165.782	−165.91	−168.494	−167.8
143.16	−94.6455	−94.0733	−94.3283	−94.6238	−97.7984	−94.4
153.16	−83.2272	−82.7287	−82.9498	−83.2071	−86.1042	−82.9
203.16	−46.4436	−46.2832	−46.3586	−46.4292	−47.684	−46.5
223.16	−37.2241	−37.1725	−37.2333	−37.2111	−37.8735	−37.3
305.00	−13.9107	−14.1748	−14.2097	−13.9013	−12.756	−15.8
601.00	12.9958	12.3132	12.2924	13.0007	16.6258	13.2
700.00	16.3830	15.6482	15.6288	16.3874	20.3131	15.8
800.00	18.8215	18.0508	18.0327	18.8255	22.9519	17.2
900.00	20.6230	19.8272	19.8104	20.6266	24.8869	19.8
1000.0	21.9923	21.179	21.1633	21.9957	26.3449	22.4
Kr						
114	−340.417	−340.306	−339.624	−339.963	−321.522	−363
124	−289.28	−289.119	−288.335	−288.832	−277.909	−306
145	−215.389	−215.278	−214.46	−215.073	−212.1	−229
153	−194.951	−194.84	−194.038	−194.658	−193.212	−201
174	−153.647	−153.536	−152.803	−153.401	−154.057	−158
203	−115.117	−115.006	−114.382	−114.915	−116.251	−117
255	−73.3739	−73.263	−72.8115	−73.221	−73.777	−75.6
305	−49.4342	−49.3233	−48.9961	−49.3096	−48.6695	−50.7
403	−22.4927	−22.3817	−22.2168	−22.4005	−19.7628	−21.9
502	−7.41916	−7.30823	−7.24396	−7.34544	−3.31801	−8.09
704	8.70138	8.81231	8.76247	8.75495	14.4076	7.09
Ne						
78.9	−13.9365			−13.9395	−12.3588	−12.6
99.2	−6.05633			−6.05877	−4.97303	−6.38
100	−5.82062			−5.82305	−4.75168	−6.0
125	−0.166542			−0.168503	0.563254	−0.157
148	3.14667			3.14499	3.68014	3.56
200	7.50606			7.50475	7.77619	7.6
300	11.1477			11.1467	11.1755	11.3
400	12.6702			12.6694	12.5749	12.8
600	13.819			13.8183	13.5941	13.8

TABLE III

The comparative values of second virial coefficients with Kihara, Lennard–Jones (12-6) potentials and Eq. (9) for Ar, Kr, Ne, CH_4, C_6H_6, C_3H_8, n-C_4H_{10} and n-C_5H_{12}

$T\,(K)$	Eq.(9)	Kihara Potential [20]	Lennard–Jones (12-6) Potential Ref. [15, 21]	Eq.(9)	Kihara Potential [20]	Lennard–Jones (12-6) Potential Ref. [15, 21]
		Ar			Kr	
100	−182.99	−182.99	−184.846	−443.157	−443.157	−404.842
200	−48.1068	−48.1068	−49.4462	−118.413	−118.413	−119.536
300	−14.9128	−14.9128	−13.8442	−51.3902	−51.3902	−50.7417
400	−0.244618	−0.244618	2.14369	−23.0879	−23.0879	−20.4085
500	7.87632	7.87632	11.0303	−7.65556	−7.65556	−3.57715
600	12.9548	12.9548	16.5811	1.96648	1.96648	6.99359
700	16.383	16.383	20.3131	8.48479	8.48479	14.1692
800	18.8215	18.8215	22.9519	13.157	13.157	19.307
900	20.623	20.623	24.8869	16.6456	16.6456	23.1311
1000	21.9923	21.9923	26.3449	19.3321	19.3321	26.0623
		Ne			CH_4	
100	−5.82062	−5.82062	−4.75168	−429.901	−429.901	−373.085
200	7.50606	7.50606	7.77619	−105.905	−105.905	−108.62
300	11.1477	11.1477	11.1755	−42.0094	−42.0094	−42.8284
400	12.6702	12.6702	12.5749	−15.4109	−15.4109	−13.604
500	13.4213	13.4213	13.2495	−1.01061	−1.01061	2.64038
600	13.819	13.819	13.5941	7.92903	7.92903	12.8362
700	14.0318	14.0318	13.7675	13.967	13.967	19.7442
800	14.1391	14.1391	13.8443	18.2851	18.2851	24.6767
900	14.1826	14.1826	13.8633	21.5034	21.5034	28.3355
1000	14.1861	14.1861	13.8465	23.978	23.978	31.1289
		C_6H_6			C_3H_8	
100	−201170.	−201164.	−100697.	−8404.14	−8404.14	−2909.57
200	−4993.56	−4993.56	−2703.32	−948.528	−948.528	−798.825
300	−1457.68	−1457.68	−861.105	−387.363	−387.363	−391.465
400	−719.333	−719.333	−464.585	−209.415	−209.415	−222.152
500	−428.552	−428.552	−305.027	−124.185	−124.185	−130.281
600	−277.3	−277.3	−220.715	−74.6287	−74.6287	−73.0332
700	−185.612	−185.612	−168.987	−42.3909	−42.3909	−34.187
800	−124.443	−124.443	−134.147	−19.8292	−19.8292	−6.25773
		$n-C_4H_{10}$			$n-C_5H_{12}$	
100	−44847.2	−44847.2	−5386.35	−169997.	−169991.	−6847.16
200	−2095.05	−2095.05	−1348.06	−4084.09	−4084.09	−1689.26
300	−711.03	−711.03	−666.946	−1176.35	−1176.35	−835.682
400	−367.573	−367.573	−394.147	−574.712	−574.712	−495.594
500	−220.857	−220.857	−248.477	−338.882	−338.882	−314.411
600	−140.911	−140.911	−158.424	−216.565	−216.565	−202.537
700	−90.9926	−90.9926	−97.562	−142.562	−142.562	−126.976
800	−57.0096	−57.0096	−53.8787	−93.2605	−93.2605	−72.7603

TABLE IV

Convergence results of expression (9) and from [20] as a function of summation limits N

N	$a^* = 0.000$ and $T^* = 100$		$a^* = 0.818$ and $T^* = 5$	
	Eq. (9)	Ref. [20]	Eq. (9)	Ref. [20]
5	0.4640692939053601	0.4640694857134132	0.6552290400583131	0.6589027966076112
10	0.4640694689727591	0.4640694689728032	0.6586984866024695	0.6587001471269023
15	0.46406946897280144	0.464069468972801	0.6587001004463544	0.6587001006874388
20	0.46406946897280144	0.46406946897280105	0.6587001006829867	0.6587001006830022
25	0.46406946897280144	0.46406946897280105	0.6587001006830024	0.6587001006830019
30	0.46406946897280144	0.464069468972801	0.6587001006830024	0.6587001006830019
35	0.46406946897280144	0.46406946897280105	0.6587001006830024	0.6587001006830018
40	0.46406946897280144	0.46406946897280105	0.6587001006830024	0.6587001006830019
45	0.46406946897280144	0.46406946897280105	0.6587001006830024	0.6587001006830018
50	0.46406946897280144	0.46406946897280105	0.6587001006830024	0.6587001006830019

TABLE V

Parameters of Lennard–Jones (12-6) potencial and Kihara potencial

Gases	Lennard–Jones (12-6) potential [15, 34]		Kihara potential [27, 28]			
	σ [Å]	ε/k_B [K]	a^*	d [Å]	σ [Å]	ε/k_B [K]
Ar	3.623	111.84	0.111	0.33570	3.36	142.10
Kr	3.895	154.87	0.144	0.44713	3.533	213.73
Ne	2.75	35.6	0.0399	0.105	2.74	39.6
CH_4	4.015	140.42	0.283	0.78569	3.562	227.13
C_6H_6	3.400	830.00	0.750	2.28686	5.336	832.00
C_3H_8	5.640	242.00	0.470	1.47427	4.611	501.89
n-C_4H_{10}	6.081	287.20	0.661	1.87714	4.717	701.15
n-C_5H_{12}	6.476	293.28	0.818	2.26277	5.029	837.82

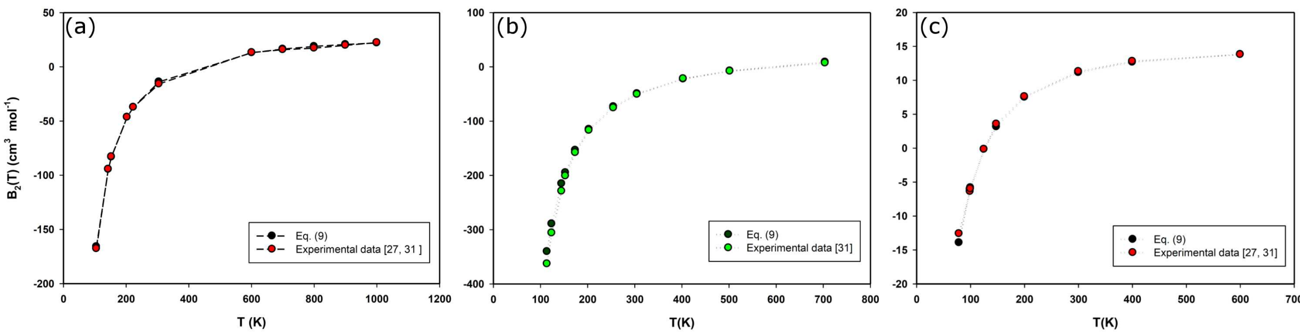

Fig. 2. The temperature dependence of second virial coefficients for: (a) Ar, (b) Kr, (c) Ne.

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