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Interaction Second Virial Coefficients of Non-spherical Molecules

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A revised analysis of the effect of long-range non-spherical terms in the intermolecular potential on the interaction second virial coefficient is presented with a preferred realistic potential functions—proposed for the molecular gases and their mixtures of noble gases—for spherical core treatment of integration in the small regions of intermolecular distances. The paper presents a contribution to the interaction second virial coefficient due to the asphericity of the molecular charge distribution. Results from calculating the non-spherical contribution to the interaction second virial coefficient with a realistic spherical core are obtained from statistical mechanics and applied to the pure system such as O_2-O_2 and H_2-H_2 and mixtures such as $N_2 + He$, $N_2 + Ar$, $O_2 + He$, $O_2 + Ar$, $H_2 + He$, $H_2 + Ne$, $H_2 + Ar$ and $H_2 + Kr$.

Key Words: Non-sphericity of molecules, Interaction potential, Second virial coefficient, Non-spherical contribution, Molecular shape.

INTRODUCTION

The virial equation of state is a standard approach used to represent experimental data of real gases[1]. This equation represents the compression factor of the mixture of interest as an infinite series expansion

$$\frac{P\overline{V}}{NkT} = 1 + \frac{B(T)}{\overline{V}} + \frac{C(T)}{\overline{V}^2} + \ldots \qquad (1)$$

where k is Boltzmann constant, and B and C are the second and third virial coefficients, respectively. By definition, the first term in the virial equation (1) represents ideal gas behaviour with subsequent terms giving corrections for real systems.

The special significance given to the virial equation of state arises primarily from the fact that the virial coefficients can be directly related to the interactions between the molecules of the system[2-6]. The second virial coefficient depends upon interactions between pairs of molecules, while the third involves the interaction energies of three molecules groupings. Thus, the evaluation of virial coefficients, principally second virial coefficient, has served as a test for model interaction potential.

The classical expression for the second virial coefficient[2] is:

$$B_2(T) = \frac{N_A}{8\pi}\int_0^{\infty} r^2\,dr \int\left[1 - \exp\left(\frac{-V(r)}{kT}\right)\right] d\omega_1\, d\omega_2 \qquad (2)$$

where $\int d\omega_1$ and $\int d\omega_2$ stand for integrations over the angular coordinates of the molecules, r is the distance between centres, and V(r) is the intermolecular potential and N_A is Avogadro's number.

It is convenient to divide intermolecular forces into three categories: (i) short range, where the potential has repulsive nature in this region and electronic exchange due to overlapping of molecular electronic shells is very substantial; (ii) intermediate range, with van der Waals minimum the actual position of which is determined by the balance between the repulsion and attraction forces; (iii) long range, where electronic exchange can be neglected and the intermolecular forces are attractive. Each individual range of distances involves its own approximations allowed to be evaluated considering the different interaction types and evaluate their contribution to the intermolecular potential[7].

The potential energy of interaction between two polyatomic molecules is usually assumed to consist of a spherically symmetric component plus a contribution due to the asphericity of the molecular charge distribution[8]. The latter contribution is conveniently divided into terms representing the classical electrostatic interaction between the two charge distributions, the anisotropy of the quantum mechanical dispersion forces and the shape of the molecular core (*i.e.*, the anisotropy of the repulsive part of the potential). Parts of the potential contribute more significantly to some properties of the molecular gas than to others. For example, the viscosity of a quadrupolar gas can usually be adequately described by a potential function consisting only of the spherical component plus the contribution due to the quadrupole moments, whereas the second virial coefficient of the same gas depends significantly on all parts of the potential function[8].

It should also be mentioned that tensor algebra is a well-known method for a molecular physicist[9–11]. Since the tensor analysis for calculation of the second virial coefficients[12] is rather complicated, it is better to adopt the method of calculation proposed by Beatie and Stockmayer[13].

An indirect method is usually used to determine intermolecular forces from virial coefficients[14, 15] due to failure of the direct approach. On the other hand many kinetic theory transport properties depend on the fact that a force exists between molecules[16–21] and only secondarily on the nature of the force.

One of the methods for the calculation of the second virial coefficients of non-spherical molecules is the perturbation procedure developed by Pople[22, 23]. They proposed that in addition to the interaction of permanent dipole, other oriented intermolecular forces such as dipole-induced dipole interaction and quadrupole may be important.

Over the past decade or so, accurate methods have been developed for describing the thermodynamic behaviour of fluid composed of simple molecules. By simple, we mean, molecules for which the most important intermolecular forces are repulsion and dispersion (van der Waals attraction), with electrostatic forces due to dipoles, quadrupole, etc. Many of the gases fall within this category. In the present study, the statistical-mechanical expression for the second virial coefficient is expanded accordingly to produce an expression that gives corrections to the spherical contribution in the form of a series that converges rapidly at high temperatures. The coefficients of the series are some integrals[8, 24–27]. These integrals are functions of temperature, which are evaluated numerically and tabulated in the present work with the explicit application of the realistic potential for the following system: O_2-O_2[28], O_2-He and O_2-Ar[29], N_2-He[30] with ESMSV potential, H_2-H_2[31], H_2-He[32] with HFD potential, H_2-Ne, H_2-Ar and H_2-Kr[33] with Buckingham-Corner and finally O_2-Kr, N_2-Kr and N_2-Ar[34] with Lennard-Jones(12-6) potential.

Methodology

If two non-spherical molecules interact, the potential energy will depend on the relative spatial orientations of the molecules as well as on their distance apart. One can write the intermolecular pair potential as the sum of a spherical part, $V_0(r)$, and a non-spherical portion V_{ns}

$$V = V_0(r) + V_{ns}(\omega_i) \tag{3}$$

in which $V_0(r)$ depends only on the intermolecular distance r, and the non-spherical potential depends also on the angles ω_i that specify the relative orientation of the molecular pair. This means that the molecules are treated as rigid rotating bodies and that the effects of vibrational degrees of freedom are left unaccounted. The effects of vibration on second virial coefficients are usually negligible for simple molecules except near the dissociation limit, which means at very high temperatures[35].

It should also mentioned that the non-spherical intermolecular potential could be written as the sum of terms that describe the long-range interactions and an additional term to describe the molecular shape[8, 24–27]:

$$V_{ns} = V_{ns}(\text{long-range}) + V_{ns}(\text{shape}) \tag{4}$$

The contributions to V_{ns} (long-range) can be conveniently divided into three parts:

$$V_{ns}(\text{long-range}) = V_{ns}(\text{electrostatic}) + V_{ns}(\text{induction}) + V_{ns}(\text{dispersion}) \tag{5}$$

The electrostatic parts, which are entirely classical interactions, arise from the interactions between permanent multi-pole moments of the molecules, such as dipole moment μ, quadrupole moment θ, and higher moments. The dominant electrostatic interactions are:

$$V_{ns}(\mu\mu) = -\frac{\mu^2}{r^3}(2c_1c_2 - s_1s_2c) \tag{6}$$

$$V_{ns}(\mu\theta) = \frac{3\mu\theta}{2r^4}(c_2 - c_1)(3c_1c_2 - 2s_1s_2c + 1) \tag{7}$$

$$V_{ns}(\theta\theta) = \frac{3\theta^2}{4r^5}\,[1 - 5c_1^2 - 5c_2^2 - 15c_1^2c_2^2 + 2(4c_1c_2 - s_1s_2c)^2] \quad (8)$$

where

$$\begin{aligned} s_1 &= \sin\theta_1 & c_1 &= \cos\theta_1 \\ s_2 &= \sin\theta_2 & c_2 &= \cos\theta_2 \\ c &= \cos(\phi_2 - \phi_1) \end{aligned} \quad (9)$$

here θ_1, θ_2, ϕ_2 and ϕ_1 are the usual angles describing the mutual orientation of two linear molecules.

The interaction between the permanent multi-pole moments of one molecule and the dipole polarizability (α_d), and quadrupole polarizability (α_q) etc., arises from quantum mechanical fluctuations of the electron distribution in an atom or molecule that gives rise to transient multi-pole moments. The dominant non-spherical induction interactions are:

$$V_{ns}(\text{induction}) = V_{ns}(\mu, \text{ind }\mu) + V_{ns}(\mu\theta, \text{ind }\mu) + V_{ns}(\theta, \text{ind }\mu) \quad (10)$$

where

$$V_{ns}(\mu, \text{ind }\mu) = -\frac{\mu^2\alpha_d}{2r^6}(3c_1^2 + 3c_2^2 - 2) - \frac{\mu^2\alpha_d^2}{r^9}(8c_1c_2 - s_1s_2c) \quad (11)$$

$$V_{ns}(\mu\theta, \text{ind }\mu) = \frac{-12\mu\theta\alpha_d}{r^7}(c_1^3 + c_2^3) \quad (12)$$

$$V_{ns}(\theta, \text{ind }\mu) = -\frac{9\theta^2\alpha_d}{8r^8}\left(4c_1^4 + 4c_2^4 + s_1^4 + s_2^4 - \frac{8}{3}\right) \quad (13)$$

The dispersion contributions arise from electrostatic interactions between transient moments in a second molecule. The dominant non-spherical dispersion interaction is

$$V_{ns}(C_6\text{ anis}) = \frac{k\overline{C}_6}{r^6}\left[1 - \frac{3}{2}(1 - k)(c_1^2 + c_2^2) - \frac{3}{2}k(2c_1c_2 - s_1s_2c)^2\right] \quad (14)$$

where $\overline{C}_6$ is the mean dispersion coefficient and κ is the anisotropy of the dipole polarizability.

$$\kappa = (\alpha_d^{\parallel} - \alpha_d^{\perp})/3\overline{\alpha}_d \quad (15)$$

in which $\alpha_d^{\parallel}$ is the polarizability along the axis of molecular symmetry while $\alpha_d^{\perp}$ is perpendicular to it and $\overline{\alpha}_d$ is the orientation averaged polarizability.

Finally, the potential energy due to molecular shape has been confined to an empirical representation as:

$$V_{ns}(\text{shape}) = \frac{A}{r^n}(3c_1^2 + 3c_2^2 - 2) \quad (16)$$

where A is a constant and n is an integer (is usually set equal to 12).

Calculations

It is shown that for light molecules and atoms and also in low temperature conditions, classical mechanics is completely inadequate to describe the molecular motion; therefore, we must use quantum mechanics instead.

Accordingly, the classical expression for the second virial coefficient, given in the preceding section, cannot be used for such quantum systems. Nevertheless, the evaluation of the virial coefficients by purely quantum mechanical methods is quite difficult. Therefore, it seems reasonable to seek for a computational method, which starts with the classical result as the first approximation and goes on by the addition of quantum correction terms. The Wigner-Kirkwood[36, 37] expansion is appropriate for this purpose. For a spherical potential, U(r), the Wigner-Krikwood expansion for the second virial coefficient yields:

$$B = B_{class} + (\eta^2/m)B_1 + (\eta^2/m)^2 B_2 + \ldots \qquad (17)$$

where B_{class} is given by eq. (3) and

$$B_1 = \frac{\pi}{6(kT)^3}\int_0^\infty U'^2 \exp\left(\frac{-U}{kT}\right) r^2\, dr$$

$$B_2 = \frac{-\pi}{6(kT)^4}\int_0^\infty \exp\left(\frac{-U}{kT}\right)\left(\frac{U''^2}{10} + \frac{U'^2}{5r^2} + \frac{U'^3}{9kT_r} + \frac{U'^4}{72(kT)^2}\right) r^2\, dr \qquad (19)$$

with

$$U' = \frac{dU}{dr}, \qquad U'' = \frac{d^2U}{dr^2}$$

We can write the intermolecular potential in terms of V_{ns} and V_0; the non-spherical part is considered as a perturbation, the exponential is then expanded in a series as follows:

$$\exp\left(\frac{-V_{ns}}{kT}\right) = 1 + \sum_{j=1}^{n} \frac{(-1)^j}{j!}\left(\frac{V_{ns}}{kT}\right)^j \qquad (20)$$

where the first term gives the spherical contribution to B(T) and the summation gives the non-spherical contribution,

$$B(T) = B_0(T) + B_{ns}(T) \qquad (21)$$

Here

$$B_0(T) = 2\pi N_A \int_0^\infty \left[1 - \exp\left(-\frac{V_0}{kT}\right)\right] r^2\, dr$$

and

$$B_{ns}(T) = -\frac{N_A}{2\Omega_0^2}\sum_{j=1}^{\infty}\frac{(-1)^j}{j!}\iiint \left(\frac{V_{ns}}{kT}\right)^j \exp\left(-\frac{V_0}{kT}\right) dr\, d\omega_1\, d\omega_2 \qquad (23)$$

The latest equation can be expressed as linear combinations of the following integrals:

$$j_n(T^*) = \frac{n-3}{2}\left(\frac{\sigma_0}{r_m}\right)^{n-3}\int_0^\infty x^{2-n}\exp\left(\frac{-V_0^*}{T^*}\right)dx \tag{24}$$

in which $T^* \equiv \frac{kT}{\varepsilon_0}$, $V_0^* \equiv \frac{V_0}{\varepsilon_0}$ and $x \equiv r/r_m$, where σ_0 is the separation at which the spherical potential is zero and ε_0 is the depth of the potential well.

Based upon the preceding paragraphs, the non-spherical contributions to the second virial coefficient for axially symmetric molecules are given as:

$$B^*_{ns}(T^*) = B^*_{ns}\text{ (electrostatic)} + B^*_{ns}\text{ (induction)} + B^*_{ns}\text{ (dispersion)}$$
$$+ B^*_{ns}\text{ (shape)} + B^*_{ns}\text{ (cross-term)} \tag{25}$$

where $B^*(T^*) = \frac{B_2}{2\pi N_A\sigma_0^3/3}$ and B^*_{ns} (cross terms) arises from a large number of cross terms resulting from multiplying out the terms $(V_{ns}/kT)^j$ in Eq. (23).

We use the notation J_n^D for J_n when the damping function is applied in the J_n integrals, *viz.*,

$$j_n^D(T^*) = \frac{n-3}{2}\left(\frac{\sigma_0}{r_m}\right)^{n-3}\int_0^\infty x^{2-n} f(x)\exp\left(\frac{-V_0^*}{T^*}\right)dx \tag{26}$$

The individual electrostatic contributions are as follows[32]:

$$B^*_{ns}(\mu\mu) = \frac{-2}{3}\left(\frac{\mu^{*2}}{T^*}\right)^2\left[J_6^D + \frac{1}{25}\left(\frac{\mu^*}{T^*}\right)^2 J_{12}^D + \ldots\right] \tag{27}$$

$$B^*_{ns}(\mu\theta) = \frac{-6}{5}\left(\frac{\mu^*\theta^*}{T^*}\right)^2\left[J_8^D + \frac{726}{3185}\left(\frac{\mu^*\theta^*}{T^*}\right)J_{16}^D + \ldots\right] \tag{28}$$

$$B^*_{ns}(\theta\theta) = \frac{-6}{5}\left(\frac{\theta^{*2}}{T^*}\right)^2\left[J_{10}^D - \frac{6}{49}\left(\frac{\theta^{*2}}{T^*}\right)^2 J_{15}^D + \ldots\right] \tag{29}$$

where $\mu^* \equiv \frac{\mu}{(\varepsilon_0\sigma_0^3)^{1/2}}$ and $\theta^* \equiv \frac{\theta}{(\varepsilon_0\sigma_0^5)^{1/2}}$

The individual induction contributions are as follows:

$$B^*_{ns}(\mu,\text{ ind }\mu) = \frac{-2}{15}\left(\frac{\mu^{*2}\alpha_d^*}{T^*}\right)^2 [J_{12}^D + 11\alpha_d^{*2}J_{18}^D + \ldots] \tag{30}$$

$$B^*_{ns}(\mu,\text{ ind }\mu) = \frac{-864}{77}\left(\frac{\mu^*\theta^*\alpha_d^*}{T^*}\right)^2 J_{14}^D + \ldots \tag{31}$$

$$B^*_{ns}(\theta,\text{ ind }\mu) = \frac{-162}{455}\left(\frac{\mu^{*2}\alpha_d^*}{T^*}\right)^2 J_{16}^D + \ldots$$

where $\alpha_d^* \equiv \frac{\overline{\alpha}_d}{\sigma_0^3}$

The dispersion contribution is:

$$B^*_{ns}(C_6 \text{ anis}) = \frac{-2}{15}\left(\frac{\kappa C_6^*}{T^*}\right)^2\left(1+\frac{19}{10}\kappa^2\right)J^D_{12}+\ldots \tag{33}$$

with $C_6^* = \dfrac{\overline{C}_6}{\varepsilon_0\sigma_0^6}$

Another contribution of the non-spherical second virial coefficients in term of J^D_n is given[23] in the following equations:

$$B^*_{ns}\text{ (shape)} = \frac{-8}{5}\left(\frac{3}{2n-3}\right)\left(\frac{A^*}{T^*}\right)^2 J^D_{2n}+\ldots \tag{34}$$

$$B^*_{ns}(\mu\times\theta) = \frac{3}{5}\left(\frac{\mu^*\theta^*}{T^*}\right)^2\left[\left(\frac{\mu^{*2}}{T^*}\right)J_{11}+\frac{24}{35}\left(\frac{\theta^{*2}}{T^*}\right)J^D_{13}+\ldots\right] \tag{35}$$

$$B^*_{ns}(\mu,\text{ ind }\mu\times\theta,\text{ ind }\mu) = \frac{-144}{385}\left(\frac{\mu^*\theta^*\alpha_d^*}{T^*}\right)^2 J^D_{14}+\ldots \tag{36}$$

$$B^*_{ns}(\theta\theta\times C_6\text{ anis}) = \frac{27}{25}\left(\frac{\theta^{*2}}{T^*}\right)\left(\frac{C_6^*}{T^*}\right)\kappa^2 J^D_{11}+\ldots \tag{37}$$

$$B^*_{ns}(\mu,\text{ ind }\mu\times C_6\text{ anis}) = \frac{-4}{15}\left(\frac{\mu^{*2}}{T^*}\right)\left(\frac{C_6^*}{T^*}\right)\alpha_d^*\kappa J^D_{12}+\ldots \tag{38}$$

$$B^*_{ns}(\theta,\text{ ind }\mu\times C_6\text{ anis}) = \frac{-144}{385}\left(\frac{\theta^*}{T^*}\right)^2\left(\frac{C_6^*}{T^*}\right)\alpha_d^*\kappa J^D_{14}+\ldots \tag{39}$$

where $A^* \equiv A/\varepsilon_0\sigma_0^n$

RESULTS AND DISCUSSION

In summary, the present study has shown that a suitable way of estimating of various contributions to the interaction second virial coefficients of fluids with linear homo-nuclear molecules and their mixtures with noble gases according to Eq. (25). The results are given in Tables 3–5. This paper has also been concerned with the evaluation of the quantum corrections to the interaction second virial coefficient of the aforesaid systems, by adopting the Wigner-Kirkwood expansion. The method provides the values of the interaction second virial coefficients of the aforementioned systems with an uncertainty commensurate with experimental accuracy. It should be mentioned that the quantum corrections on the interaction second virial coefficients are also considered in our calculation by the eqs. (17–19). Now, the origin of the non-spherical contributions in the interaction second virial coefficients is clear. On the other hand, the physical effects appear to distinguish between one kind of force and another. The substances in Tables 3–5 are particularly interesting. They belong to a class of molecules, often called "linear", whose intermolecular potential is usually assumed largely anisotropic. It is apparent that they are far from spherical. The interaction second virial coefficient of these pure and mixture systems differs from those of an assembly of spherical molecules. Finally, not only the nature of these various kinds of forces is not obscure, but also their physical effects are clear.

TABLE-1
EXAMPLE OF EFFECT OF DAMPING ON THE CALCULATED NON-SPHERICAL CONTRIBUTION TO THE INTERACTION SECOND VIRIAL COEFFICIENT H_2-He. THE CORE POTENTIAL IS HFD-B

Contribution	$T^* = 1$		$T^* = 5$	
	Undamped	Damped	Undamped	Damped
B^*ns (θ, ind μ)	-4.37×10^{-6}	-3.48×10^{-6}	-2.98×10^{-7}	-1.96×10^{-7}
B^*ns (C_6 anis)	-6.28×10^{-3}	-5.18×10^{-3}	-2.84×10^{-4}	-2.02×10^{-4}
B^*ns (θ, ind μ × C_6 anis)	-2.85×10^{-4}	-2.30×10^{-4}	-1.57×10^{-5}	-1.07×10^{-5}
B_0 (spherical)	−37.7729		+12.7506	

TABLE-2
SAME AS TABLE-1 FOR H_2. THE CORE POTENTIAL IS HFD-A

Contribution	$T^* = 1$		$T^* = 5$	
	Undamped	Damped	Undamped	Damped
B^*ns (θθ)	−0.19072	−0.16754	-7.72×10^{-3}	-6.07×10^{-3}
B^*ns (θ, ind)	-3.04×10^{-5}	-2.11×10^{-5}	-3.24×10^{-6}	-4.64×10^{-6}
B^*ns (C_6 anis)	-1.28×10^{-2}	-1.10×10^{-2}	-4.53×10^{-4}	-6.04×10^{-4}
B^*ns (θθ × C_6 anis)	-1.24×10^{-2}	1.08×10^{-2}	4.07×10^{-4}	5.30×10^{-4}
B^*ns (θ, ind μ × C_6 anis)	-1.53×10^{-3}	-1.30×10^{-3}	-6.46×10^{-5}	-8.93×10^{-5}
B_0 (spherical)	−50.9576		9.117901	

TABLE-3
THE CALCULATED VALUES OF NON-SPHERICAL CONTRIBUTION TO THE INTERACTION SECOND VIRIAL B^*_{ns} (T^*) FOR H_2-NOBLE GAS MIXTURES

T*	H_2-H_2	H_2-He	H_2-Ne	H_2-Ar	H_2-Kr
0.5	−1.304	-4.29×10^{-2}	-4.40×10^{-2}	-4.20×10^{-2}	-4.37×10^{-2}
1	−0.169	-5.41×10^{-3}	-5.47×10^{-3}	-5.29×10^{-3}	-5.50×10^{-3}
2	−0.035	-1.13×10^{-3}	-1.10×10^{-3}	-1.10×10^{-3}	-1.15×10^{-3}
3	-1.56×10^{-2}	-5.19×10^{-4}	-4.87×10^{-4}	-5.01×10^{-4}	-5.23×10^{-4}
4	-9.19×10^{-3}	-3.11×10^{-4}	-2.85×10^{-4}	-2.99×10^{-4}	-3.13×10^{-4}
5	-6.18×10^{-3}	-2.13×10^{-4}	-1.91×10^{-4}	-2.04×10^{-4}	-2.14×10^{-4}
6	-4.51×10^{-3}	-1.58×10^{-4}	-1.39×10^{-4}	-1.51×10^{-4}	-1.58×10^{-4}
7	-3.47×10^{-3}	-1.23×10^{-4}	-1.07×10^{-4}	-1.18×10^{-4}	-1.23×10^{-4}
8	-2.78×10^{-3}	-1.00×10^{-4}	-8.54×10^{-5}	-9.54×10^{-5}	-9.98×10^{-5}
9	-2.28×10^{-3}	-8.35×10^{-5}	-7.03×10^{-5}	-7.94×10^{-5}	-8.31×10^{-5}
10	-1.93×10^{-3}	-7.13×10^{-5}	-5.92×10^{-5}	-6.76×10^{-5}	-7.07×10^{-5}

TABLE-4
SAME AS TABLE-3 FOR N_2-NOBLE GAS MIXTURES

T*	N_2-He	N_2-Ar	N_2-Kr
0.5	-7.75×10^{-2}	-0.27	-2.18×10^{-2}
1	-1.01×10^{-2}	3.37×10^{-2}	-2.75×10^{-3}
2	-2.22×10^{-3}	-7.03×10^{-2}	-5.76×10^{-4}
3	-1.05×10^{-3}	-3.21×10^{-3}	-2.64×10^{-4}
4	-6.46×10^{-4}	-1.92×10^{-3}	-1.58×10^{-4}
5	-4.50×10^{-4}	-1.31×10^{-3}	-1.09×10^{-4}
6	-3.40×10^{-4}	-9.72×10^{-4}	-8.05×10^{-5}
7	-2.68×10^{-4}	-7.58×10^{-4}	-6.29×10^{-5}
8	-2.20×10^{-4}	-6.14×10^{-4}	-5.10×10^{-5}
9	-1.85×10^{-4}	-5.11×10^{-4}	-4.25×10^{-5}
10	-1.59×10^{-4}	-4.35×10^{-4}	-3.62×10^{-5}

TABLE-5
SAME AS TABLE-3 FOR O_2-NOBLE GAS MIXTURES

T*	O_2-O_2	O_2-He	O_2-Ar	O_2-Kr
0.5	-3.56×10^{-1}	-8.87×10^{-2}	-1.61×10^{-1}	-5.49×10^{-2}
1	-4.57×10^{-2}	-1.29×10^{-2}	-2.05×10^{-2}	-6.91×10^{-3}
2	-9.84×10^{-3}	-3.16×10^{-3}	-4.30×10^{-3}	-1.44×10^{-3}
3	-4.63×10^{-3}	-1.60×10^{-3}	-1.96×10^{-3}	-6.59×10^{-4}
4	-2.84×10^{-3}	-1.03×10^{-3}	-1.18×10^{-3}	-3.94×10^{-4}
5	-1.99×10^{-3}	-7.43×10^{-4}	-8.09×10^{-4}	-2.69×10^{-4}
6	-1.50×10^{-3}	-5.78×10^{-4}	-6.03×10^{-4}	-1.99×10^{-4}
7	-1.19×10^{-3}	-4.72×10^{-4}	-4.75×10^{-4}	-1.55×10^{-4}
8	-9.83×10^{-4}	-3.99×10^{-4}	-3.88×10^{-4}	-1.25×10^{-4}
9	-8.32×10^{-4}	-3.45×10^{-4}	-3.27×10^{-4}	-1.05×10^{-4}
10	-7.19×10^{-4}	-3.05×10^{-4}	-2.82×10^{-4}	-8.90×10^{-5}

Conclusion

In the present study the interaction second virial coefficients of some diatomic gases have been calculated using proposed realistic potential for O_2-O_2, H_2-H_2 and mixtures such as $N_2 + He$, $N_2 + Ar$, $N_2 + Kr$, $O_2 + He$, $O_2 + Ar$, $O_2 + Kr$, $H_2 + He$, $H_2 + Ne$, $H_2 + Ar$ and $H_2 + Kr$ as core potential for the calculation of the non-spherical contribution to the interaction second virial coefficients. As the other investigators have observed the interaction second virial coefficient is also quite sensitive to the choice of the pair-interaction potential energy function[1-4], hence, the unique novelty of the present study seems to describe an interesting example of the application of the proposed realistic potential to largely anisotropic systems which appears to be intuitively reasonable. As the figures 1–3 show, the

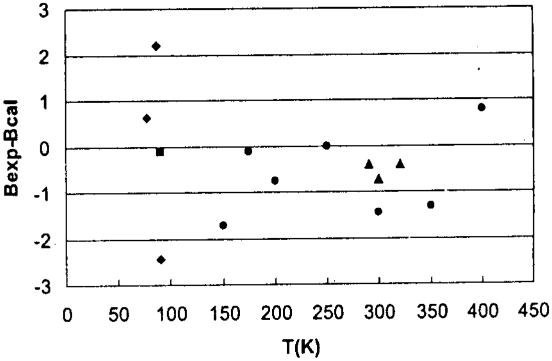

Fig. 1. Deviation of the calculated values of the interaction second virial coefficients (cc/mole) for pure and mixtures from the experimental values. $O_2 + He$: (◆) Ref. [46], (■) Ref. [45]; $O_2 + Ar$: (▲) Ref. [46]; and of O_2-O_2: (●) Ref. [46]

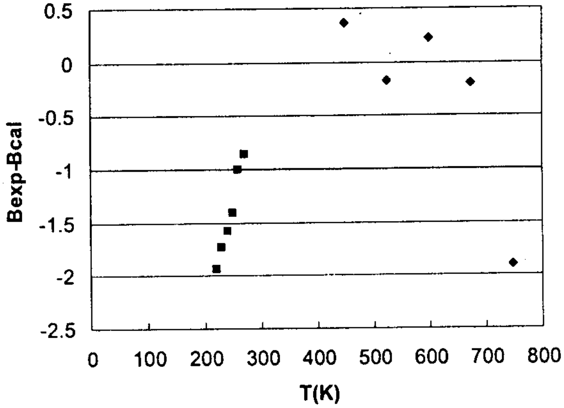

Fig. 2. Same as Fig. 1. $N_2 + He$: (◆) Ref. [45]; $N_2 + Ar$: (■) Ref. [45]

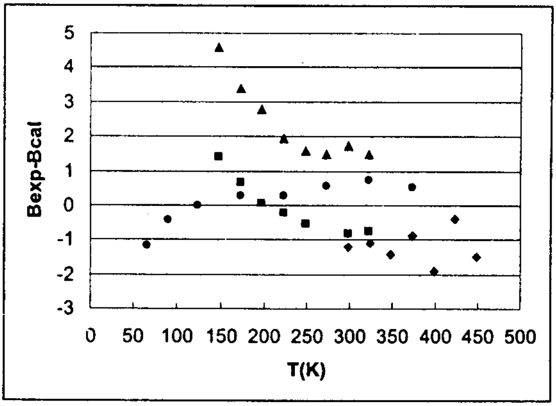

Fig. 3. Same as Fig. 1. H_2 + He: (♦) Ref. [45]; H_2 + Ne (■) Ref. [45]; H_2 + Ar: (▲) Ref. [45]; and H_2-H_2: (•) Ref. [45]

errors, within 4% cc/mol are in good agreement with experimental uncertainty for a wide range of temperatures.

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