Second Virial Coefficients and Transport Properties of Hexafluoride Gases from an Improved Intermolecular Potential

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Second virial coefficients and a large number of Chapman-Cowling collision integrals were calculated for gases obeying an improved intermolecular potential proposed by Aziz et al. [J. Chem. Phys. **94,** 1034 (1991)]. The results are tabulated for a large reduced temperature range, kT/ε from 0.1 to 100. The treatment was entirely classical, and no corrections for quantum effects were made. The higher approximations to the transport coefficients were also calculated and tabulated for the same temperature range. These results should be applicable to characterize the bulk properties of various spherical molecules, especially to predict gaseous transport properties. Evaluation of the potential parameters for uranium hexafluoride, together with fitting to second virial coefficient, viscosity, thermal conductivity and self-diffusion data are also presented. This potential appears to have the best overall predictive ability for gaseous hexafluoride data.

1. Introduction

Several effective isotropic pair potential functions have been proposed to characterize the bulk properties of quasi-spherical molecules, in particular the hexafluorides [1–4]. Generally these potentials have steeper repulsive walls than those which describe the rare gases.

Recently Aziz et al. [5] have constructed a Morse-Morse-Spline-van der Waals (MMSV) potential which incorporates the determination of the C_6 dispersion coefficient [6] and satisfactorily correlates second virial coefficient and viscosity data of sulfur hexafluoride. None of the potential functions previously proposed in literature could predict these properties simultaneously.

The Morse-Morse-Spline-van der Waals (MMSV) functional form is given by

$$V(r) = \varepsilon\, V^*(x), \qquad (1)$$

where

$$\begin{aligned}
V^*(x) &= \exp[-2\,\beta_1(x-1)] - 2\exp[-\beta_1(x-1)], & 0 \le x \le 1\\
&= \exp[-2\,\beta_2(x-1)] - 2\exp[-\beta_2(x-1)], & 1 \le x \le x_1\\
&= a_1 + (x-x_1)\,\{a_2 + (x-x_2)\,[a_3 + (x-x_1)\,a_4]\}, & x_1 \le x \le x_2\\
&= -\left(\frac{C_6}{x^6} + \frac{C_8}{x^8} + \frac{C_{10}}{x^{10}}\right), & x \ge x_2, \qquad (2)
\end{aligned}$$

and $x = r/r_{\mathrm{m}}$.

The significance of the symbols in the above Equation is given in [5].

The aim of the present paper is to calculate the reduced second virial coefficients, the Enskog-Chapman collision integrals and the higher approximations to the transport coefficients for the MMSV potential, because these results should be applicable to characterize the bulk properties of various spherical molecules, especially of hexafluorides. At the same time, the determination of the uranium hexafluoride potential parameters for this more realistic potential was achieved, UF_6 being the gaseous compound of uranium used for the enrichment of ^{235}U.

2. Second Virial Coefficients

The equation of state of any gas [7] may be written in virial form

$$\frac{P\,\tilde{V}}{RT} = 1 + \frac{B(T)}{\tilde{V}} + \frac{C(T)}{\tilde{V}^2} + \frac{D(T)}{\tilde{V}^3} + \ldots, \qquad (3)$$

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where the coefficients $B(T)$, $C(T)$, $D(T)$, ... are called the second, third, fourth ... virial coefficients and are functions of temperature, T, and the nature of the material under investigation.

According to classical statistical mechanics, the second virial coefficient, $B(T)$, may be related [7] to the intermolecular pair potential $V(r)$ by

$$B(T) = -2\pi N_A \int_0^\infty [\exp(-V(r)/kT) - 1]\, r^2 \,\mathrm{d}r, \tag{4}$$

N_A being Avogadro's number.

It is convenient to introduce the reduced quantities:

$$r^* = \frac{r}{\sigma}, \quad V^*(r^*) = \frac{V(r)}{\varepsilon}, \quad T^* = \frac{kT}{\varepsilon} \tag{5}$$

and

$$B^*(T^*) = \frac{B(T)}{b_0}, \quad b_0 = \frac{2}{3}\pi N_A \sigma^3, \tag{6}$$

where ε and σ represent potential parameters. The reduced second virial coefficient, $B^*(T^*)$ is a function of the reduced temperature T^*, having the form

$$B^*(T^*) = -3 \int_0^\infty [\exp(-V(r^*)/T^*) - 1]\, r^{*2} \,\mathrm{d}r^*, \tag{7a}$$

or

$$B^*(T^*) = -\frac{1}{T^*} \int_0^\infty \exp(-V(r^*)/T^*) \frac{\mathrm{d}V(r^*)}{\mathrm{d}r}\, r^{*3} \,\mathrm{d}r^*. \tag{7b}$$

To estimate $B^*(T^*)$, a classical method was used (trapeze rule combined with Romberg's principle). This method belongs to the mathematical library Control Data Corporation (CDC) [8, 9]. At a requested accuracy, for a convergence at least in the sixth decimal, the mean number of bisections was seven, the maximum number of these being thirty for every region of integration. For each integral we divided the range of integration into four regions (I_1, I_2, I_3, I_4) of r^*, corresponding to the regions where the Morse-Morse-Spline-van der Waals (MMSV) potential functional form is defined (see (2)). Since for different values of the reduced temperature, T^*, the integrand varies much especially for the (0, 1) region, we again divided this region as follows: $(0, \alpha) \rightarrow I_{10}$, $(\alpha, x_0) \rightarrow I_{11}$ and $(x_0, 1) \rightarrow I_{12}$, x_0 being the value where $V(r^*) = 0$. The used the following values of α: $\alpha = 0.974$ for $T^* \leq 1$; $\alpha = 0.958$ for $T^* \leq 10$; $\alpha = 0.938$ for $T^* \leq 100$. The parameter a was introduced for accuracy reasons.

In terms of the MMSV potential, values obtained for $B^*(T^*)$ are given in Table 1 for the reduced temperature ranging from 0.3 to 100.

Table 1. The reduced second virial coefficients, $B(T^*)$, for the MMSV potential.

T^*	$B(T^*)$	T^*	$B(T^*)$
0.3	−13.68226	4.5	0.65954
0.4	−6.52175	5.0	0.69119
0.5	−3.92936	6.0	0.73753
0.6	−2.63982	7.0	0.76970
0.7	−1.87834	8.0	0.79322
0.8	−1.37851	9.0	0.81107
0.9	−1.02621	10.0	0.82504
1.0	−0.76492	12.0	0.84532
1.2	−0.40382	14.0	0.85918
1.4	−0.16643	16.0	0.86913
1.6	0.00131	18.0	0.87653
1.8	0.12604	20.0	0.88217
2.0	0.22236	40.0	0.90230
2.5	0.38823	60.0	0.90480
3.0	0.49355	80.0	0.90398
3.5	0.56619	100.0	0.90224
4.0	0.61921		

Corresponding states behavior of the second virial coefficient is expected for substances which have similar potential energy functions.

3. Transport Properties

Information concerning intermolecular forces may be obtained from the temperature variation of gaseous transport coefficients by means of the theory developed by Enskog and by Chapman [10].

Such information is useful in correlating other properties of gases, as well as properties of liquid and solid states.

According to [10], the transport phenomena depend on the intermolecular potential through collisions of single pairs of molecules, and the only feature of a collision [7, 10, 11], which it is necessary to consider is the angle of deflection χ, through which the relative velocity vector of a pair of molecules under consideration is rotated by the collision.

The reduced transport cross-section $Q^{(1)*}(E^*)$ is defined by the equation [10]

$$Q^{(1)*}(E^*) = 2\left[1 - \frac{1 + (-1)^l}{2(1+l)}\right]^{-1} \int_0^\infty (1 - \cos^l \chi)\, b^* \,\mathrm{d}b^*, \tag{8}$$

where $E^* = E/\varepsilon$, $b^* = b/\sigma$, $r^* = r/\sigma$ and $V^* = V/\varepsilon$ are reduced quantities. ε and σ are the potential parameters, E is the relative kinetic energy of collision and b is the impact parameter.

Finally, the reduced collision integrals, which directly determine the transport properties, are

$$\Omega^{(l,s)*}(T^*) = [(s+1)!\, T^{*\,s+2}]^{-1} \int_0^\infty Q^{(l)*}(E^*) \cdot e^{-E^*/T^*} E^{*\,s+1}\, \mathrm{d}E^*, \qquad (9)$$

where $T^* = kT/\varepsilon$ is the reduced temperature.

The cross sections have been reduced by dividing by $\pi\sigma^2$, and the collision integrals are divided by their values for rigid spheres of diameter σ. Thus, $Q^{(1)*}(E^*)$ and $\Omega^{(l,s)*}(T^*)$ are unity for rigid spheres.

The values of the transport coefficients [7, 11] may be expressed as infinite series. Fortunately, the convergence is rapid and very few terms are needed.

The coefficient of viscosity, η, of a pure gas, in μP, is [7, 12]

$$\eta = \frac{26.693\sqrt{M \cdot T}}{\sigma^2\, \Omega^{(2,2)*}(T^*)} \cdot f_\eta^{(n)}, \qquad (10)$$

where M is the molecular weight and the infinite series $f_\eta^{(n)}$ is a complicated function of the collision integrals. The expressions for the first three terms of f_η are given in terms of the collision integrals in [10, 11].

The coefficient of thermal conductivity, λ, of a pure gas, in cal · cm^{-1} · s^{-1} · grad^{-1}, is [7, 13]

$$\lambda = \frac{1.9891 \cdot 10^{-4}\sqrt{T/M}}{\sigma^2\, \Omega^{(2,2)*}(T^*)} \cdot f_\lambda^{(n)}. \qquad (11)$$

The application of this expression for polyatomic gases involves the Eucken correction [13], and so (11) becomes

$$\lambda' = \lambda\left(\frac{4}{15} \cdot \frac{C_p}{\gamma R} + \frac{3}{5}\right), \qquad (12)$$

where λ is the adiabatic coefficient, C_p is the molar heat capacity at constant pressure and R is the gas constant per mole.

The third approximation to f_λ is given in [10, 11]. It is also a very complicated function of the collision integrals.

The self-diffusion coefficient D of a pure gas, in cm^2/s, is [7, 12]

$$D = \frac{2.628 \cdot 10^{-3} \cdot T^{3/2}}{M^{1/2}\, p\, \sigma^2\, \Omega^{(1,1)*}(T^*)} \cdot f_D^{(n)}, \qquad (13\,\mathrm{a})$$

and in μP it is [7, 13]

$$D\varrho = \frac{2.628 \cdot 10^{-3}\sqrt{T \cdot M}}{R\, \sigma^2\, \Omega^{(1,1)*}(T^*)} \cdot f_D^{(n)}, \qquad (13\,\mathrm{b})$$

where p is the pressure and ϱ the density.

The second approximation to the quantity f_D appearing in (13 a) and (13 b) is given [10, 11] by

$$f_D^{(2)} = \frac{1}{1-\Delta}, \qquad (14)$$

where

$$\Delta = \frac{(6C^* - 5)^2}{(55 - 12B^* + 16A^*)}, \qquad (15)$$

and

$$A^* = \frac{\Omega^{(2,2)*}}{\Omega^{(1,1)*}}, \quad B^* = \frac{5\,\Omega^{(1,2)*} - 4\,\Omega^{(1,3)*}}{\Omega^{(1,1)*}},$$

$$C^* = \frac{\Omega^{(1,2)*}}{\Omega^{(1,1)*}}. \qquad (16)$$

Except for very simple and physically unrealistic potential forms, the calculation of collision integrals involves extensive numerical integrations.

Clenshaw and Curtiss have described [14] a method to estimate definite integrals through the integrand development in a finite series of Cebishev polynomials and integration of each term of the series.

This is an efficient evaluation method because of its accuracy, simplicity and easy error evaluation. Therefore we chose for the calculation of the reduced collision integrals the program catalog number ACQN (authors O'Hara and Smith [15]) adapted to run in double precision on IBM computers by Neufeld and Aziz [16], and subsequent adapted by us to run on PC computers.

The inherent computational error is estimated to be of the order of 0.1%, except for very small T^*, where it may be larger.

In terms of MMSV potential, the values of the reduced collision integrals are given in Table 2 for T^* from 0.1 to 100.

These reduced collision integrals, calculated for the MMSV potential, vary relatively slowly with T^*, compared with the 12-6 Lennard-Jones potential.

Table 3 presents the functions $f^{(n)}$ giving higher approximations to the transport coefficients for the pure gases. The superscripts indicate that these are the third approximation for the viscosity and thermal conductivity and the second approximation for the self-diffusion coefficient.

Table 2. The reduced collision integrals for the MMSV potential.

T^*	$\Omega^{(1,1)*}$	$\Omega^{(1,2)*}$	$\Omega^{(1,3)*}$	$\Omega^{(1,4)*}$	$\Omega^{(1,5)*}$	$\Omega^{(2,2)*}$	$\Omega^{(2,3)*}$	$\Omega^{(2,4)*}$	$\Omega^{(2,5)*}$
0.1	2.5967	2.3537	2.2052	2.0986	2.0267	2.7826	2.5741	2.4259	2.3123
0.2	2.1754	2.0083	1.8963	1.8046	1.7205	2.3055	2.1707	2.0825	2.0182
0.3	1.9774	1.8169	1.6910	1.5792	1.4809	2.1114	1.9988	1.9067	1.8213
0.4	1.8345	1.6653	1.5301	1.4184	1.3319	1.9769	1.8538	1.7407	1.6361
0.5	1.7186	1.5450	1.4123	1.3128	1.2401	1.8597	1.7222	1.5998	1.4947
0.6	1.6234	1.4504	1.3286	1.2410	1.1822	1.7572	1.6113	1.4895	1.3921
0.7	1.5443	1.3787	1.2664	1.1919	1.1432	1.6656	1.5208	1.4046	1.3187
0.8	1.4795	1.3218	1.2206	1.1566	1.1153	1.5890	1.4468	1.3403	1.2648
0.9	1.4243	1.2761	1.1861	1.1301	1.0947	1.5238	1.3871	1.2907	1.2242
1.0	1.3791	1.2394	1.1592	1.1095	1.0789	1.4678	1.3392	1.2515	1.1930
1.2	1.3078	1.1861	1.1196	1.0803	1.0562	1.3787	1.2674	1.1949	1.1481
1.4	1.2539	1.1487	1.0928	1.0605	1.0406	1.3144	1.2170	1.1561	1.1179
1.6	1.2138	1.1207	1.0735	1.0462	1.0293	1.2657	1.1802	1.1284	1.0962
1.8	1.1832	1.0997	1.0591	1.0354	1.0205	1.2277	1.1524	1.1077	1.0799
2.0	1.1584	1.0833	1.0479	1.0268	1.0135	1.1978	1.1307	1.0916	1.0673
2.5	1.1131	1.0553	1.0281	1.0114	1.0005	1.1446	1.0935	1.0636	1.0447
3.0	1.0837	1.0372	1.0150	1.0009	0.9913	1.1107	1.0698	1.0453	1.0295
3.5	1.0638	1.0244	1.0055	0.9929	0.9844	1.0874	1.0531	1.0322	1.0185
4.0	1.0492	1.0147	0.9982	0.9866	0.9789	1.0703	1.0408	1.0221	1.0100
4.5	1.0377	1.0071	0.9922	0.9816	0.9743	1.0570	1.0310	1.0143	1.0032
5.0	1.0284	1.0010	0.9874	0.9774	0.9704	1.0465	1.0231	1.0078	0.9976
6.0	1.0142	0.9913	0.9797	0.9706	0.9642	1.0306	1.0112	0.9978	0.9889
7.0	1.0040	0.9843	0.9738	0.9653	0.9594	1.0192	1.0023	0.9904	0.9825
8.0	0.9962	0.9787	0.9690	0.9611	0.9555	1.0104	0.9954	0.9847	0.9775
9.0	0.9899	0.9741	0.9651	0.9575	0.9523	1.0035	0.9900	0.9801	0.9735
10.0	0.9849	0.9702	0.9617	0.9545	0.9495	0.9978	0.9856	0.9763	0.9702
12.0	0.9771	0.9640	0.9564	0.9497	0.9450	0.9892	0.9786	0.9704	0.9650
14.0	0.9711	0.9592	0.9522	0.9458	0.9414	0.9828	0.9735	0.9661	0.9619
16.0	0.9662	0.9554	0.9487	0.9427	0.9385	0.9778	0.9694	0.9627	0.9582
18.0	0.9623	0.9521	0.9459	0.9401	0.9361	0.9739	0.9662	0.9599	0.9558
20.0	0.9590	0.9494	0.9434	0.9378	0.9339	0.9706	0.9636	0.9577	0.9538
40.0	0.9408	0.9339	0.9294	0.9247	0.9218	0.9543	0.9502	0.9460	0.9437
60.0	0.9323	0.9263	0.9223	0.9179	0.9152	0.9477	0.9445	0.9408	0.9388
80.0	0.9268	0.9213	0.9175	0.9132	0.9105	0.9437	0.9409	0.9374	0.9354
100.0	0.9228	0.9176	0.9139	0.9096	0.9070	0.9409	0.9382	0.9347	0.9327

Table 3. Functions for calculating the higher approximations to the transport coefficients of pure substances for the MMSV potential. $[\eta]_3=[\eta]_1\, f_\eta^{(3)}$, $[\lambda]_3=[\lambda]_1\, f_\lambda^{(3)}$, $[D]_2=[D]_1\, f_D^{(2)}$.

T^*	$f_\eta^{(3)}$	$f_\lambda^{(3)}$	$f_D^{(2)}$
0.1	1.00249	1.00375	1.00330
0.2	1.00433	1.00652	1.00500
0.3	1.00528	1.00772	1.00456
0.4	1.00429	1.00605	1.00346
0.5	1.00291	1.00404	1.00269
0.6	1.00194	1.00272	1.00225
0.7	1.00157	1.00223	1.00219
0.8	1.00129	1.00191	1.00225
0.9	1.00123	1.00187	1.00243
1.0	1.00137	1.00209	1.00264
1.2	1.00189	1.00291	1.00334
1.4	1.00249	1.00381	1.00423
1.6	1.00317	1.00484	1.00498
1.8	1.00390	1.00593	1.00568
2.0	1.00459	1.00696	1.00639
3.0	1.00763	1.01137	1.00945
4.0	1.00943	1.01390	1.01106
5.0	1.01053	1.01544	1.01212
10.0	1.01287	1.01867	1.01425
100.0	1.01526	1.02194	1.01602

4. Evaluation of the UF_6-Parameters for the MMSV Potential

The uranium hexafluoride potential parameters together with transport properties and virial coefficients have already been evaluated by the Lennard-Jones 12-6 [17–20] and 13.58-6 [12] potentials, the hard-core potential of Kihara [21], and the modified Buckingham (Exp-Six) potential [22–24]. It was found that none of these potentials could satisfactorily predict all properties simultaneously. For this reason we tried to determine the uranium hexafluoride potential parameters for a more realistic potential form than has been used previously, the Morse-Morse-Spline-van der Waals (MMSV) potential [5].

To find a single set of potential parameters which could predict the viscosity, thermal conductivity, self-diffusion, and second virial coefficients simultaneously, a large assortment of literature data was used.

Second virial coefficients of uranium hexafluoride from 320 to 592,2 K have been measured by Malyshev [17, 18], Morizot [13, 19] and Heintz [12].

Viscosity data in the temperature range 313.16–473.16 K have been reported by Myerson [25], Ostorero [26] and Morizot [17].

It has been the custom to ignore thermal conductivity data in assessing the merits of potentials in view of the fact that, like viscosity, it depends on the collision integral $\Omega^{(2,2)*}$ and that viscosity can be measured to a higher degree of accuracy than thermal conductivity. Despite of this, we have considered the thermal conductivity data of De Witt [27] and Schimid [21], measured in the temperature range 273.16–433.16 K. The constant pressure heat capacity data were taken from [28].

The self-diffusion data cover the temperature range from 273.16 to 333.16 K [29–31]. With an uncertainty of 2–3 per cent and more [29], these data would not act as an adequate discriminator for potential parameters. A treatment of self-diffusion is only included for completeness.

The method suggested by Morizot [13] was used for evaluating the best set of potential parameters of uranium hexafluoride, for MMSV potential.

Firstly, from (6), (10), (11), and (13b), Tables 1, 2, and 3, and the measured virial coefficient-, viscosity-, thermal conductivity- and self-diffusion-data we have obtained the curves $\sigma = \sigma(\varepsilon/k)$. For each value of ε/k in the range 350–850 K we minimized the standard mean deviation of the difference between the measured and calculated values. Finally, we determined the $\sigma_{\text{optimum}}(\varepsilon/k)$ curves. The best set of potential parameters will be placed on the intersection of all curves (see Figure 1). Since the $\sigma_{\text{optimum}}(\varepsilon/k)$ curves for the transport properties are parallel, the virial coefficients play the most important role as discriminator for potential parameters.

The potential parameters of uranium hexafluoride for the MMSV potential established by us are: $\varepsilon/k = 764 \pm 2$ K and $\sigma = 5.01 \pm 0.1$ Å. In Table 4 we present our results together with the potential parameters of uranium hexafluoride, for Lennard-Jones, Kihara and modified (exp-six) Buckingham potentials.

With these potential parameters we determined the percentage deviation of the experimental data from the predictions of the MMSV potential. For the transport properties we have: the viscosity data, Ostorero [26] 0.2–3.5%, Morizot [19] 1–2%, Myerson [25] 0.5–4.5%; the self-diffusion data, Gallaway [31] 2–3%,

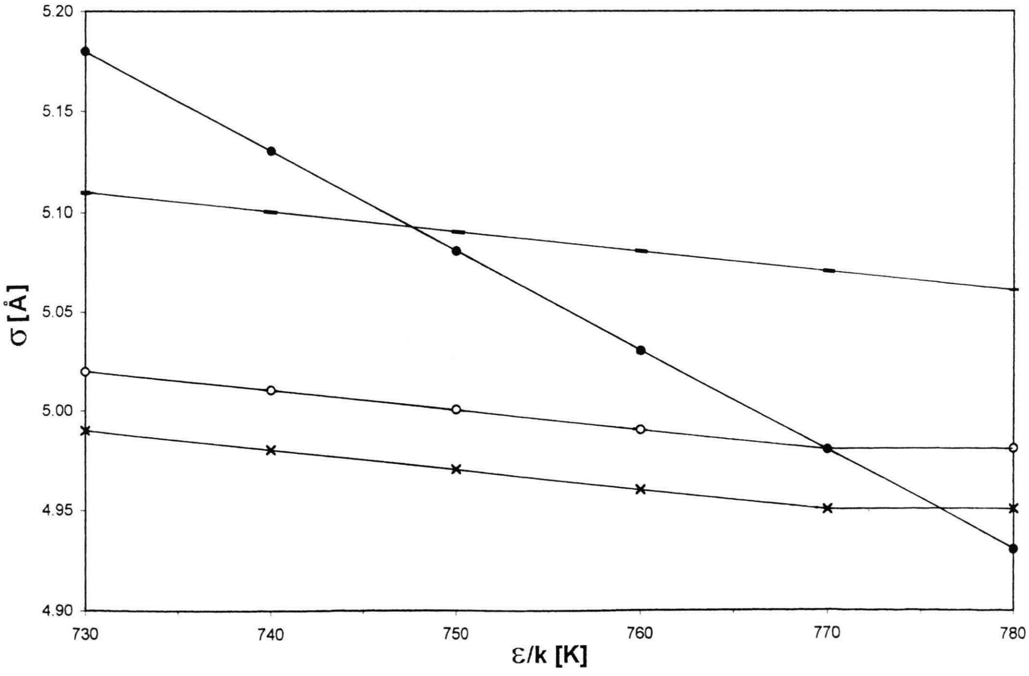


Fig. 1. The ε/k dependence of σ_{optimum}, calculated from: viscosity (×), thermal conductivity (○), self-diffusion (–) and second virial coefficient (●) average data. Zoom between 4.9–5.2 Å and 730–780 K.

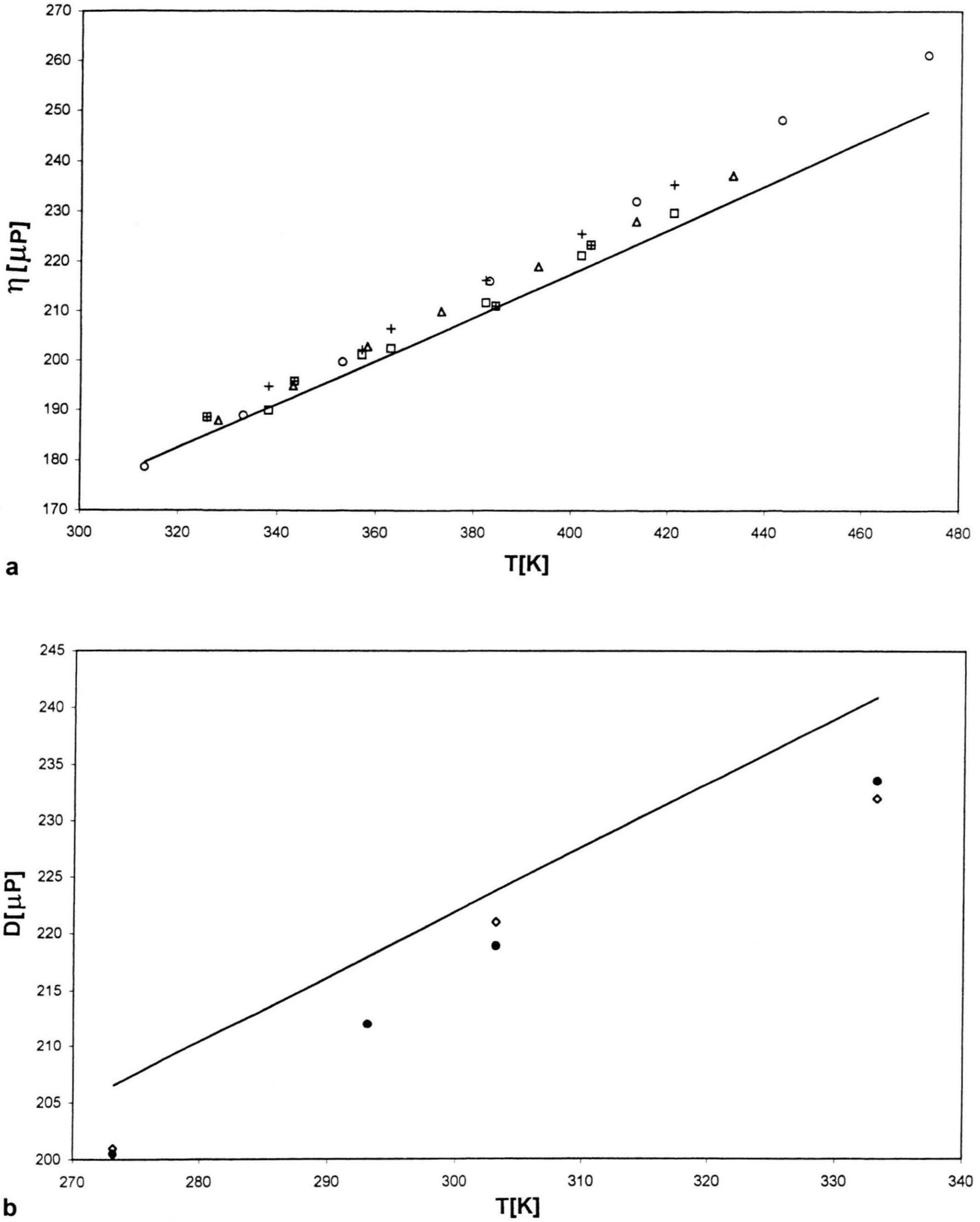
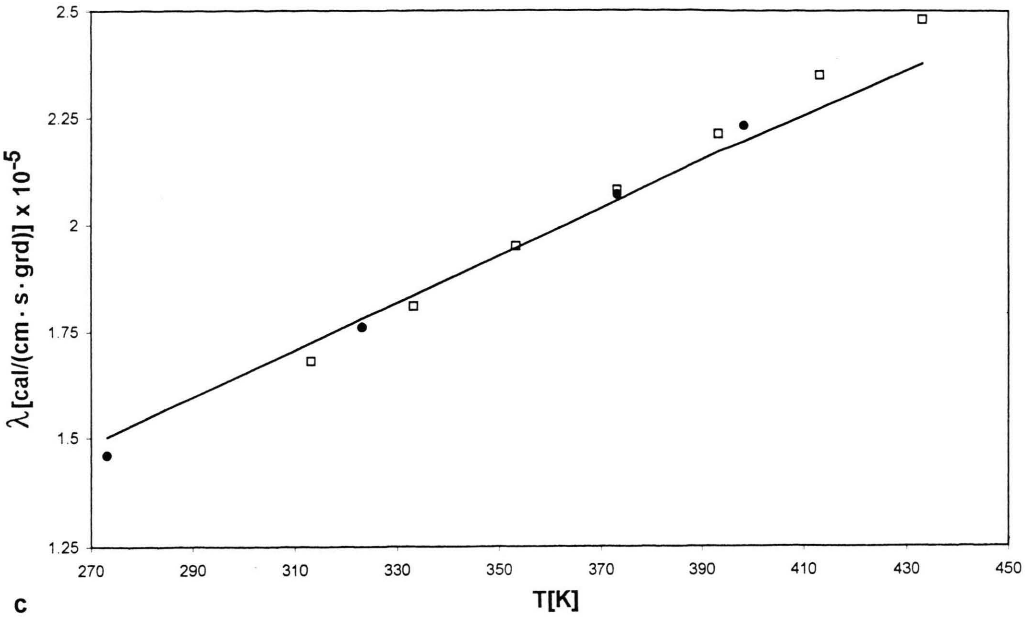


Fig. 2a, b

Fig. 2. The temperature dependence of experimental data and calculated using an MMSV potential for UF_6: a) viscosity, (□) Ostorero [26], (+) Ostorero [26], (△) Morizot [19], (○) Myerson [25]; b) self-diffusion, (●) Gallaway [31], (◇) Brown [30]; c) thermal conductivity, (□) Schimid [22], (●) De Witt [27]; d) second virial coefficient: (◇) Malyshev [17], (▲) Malyshev [18], (□) Morizot [19], (×) Morizot [13], (■) Heintz [12].


2.5
2.25
2
1.75
1.5
1.25
λ[cal/(cm · s · grd)] x 10^{-5}
270
290
310
330
350
370
390
410
430
450
T[K]
c

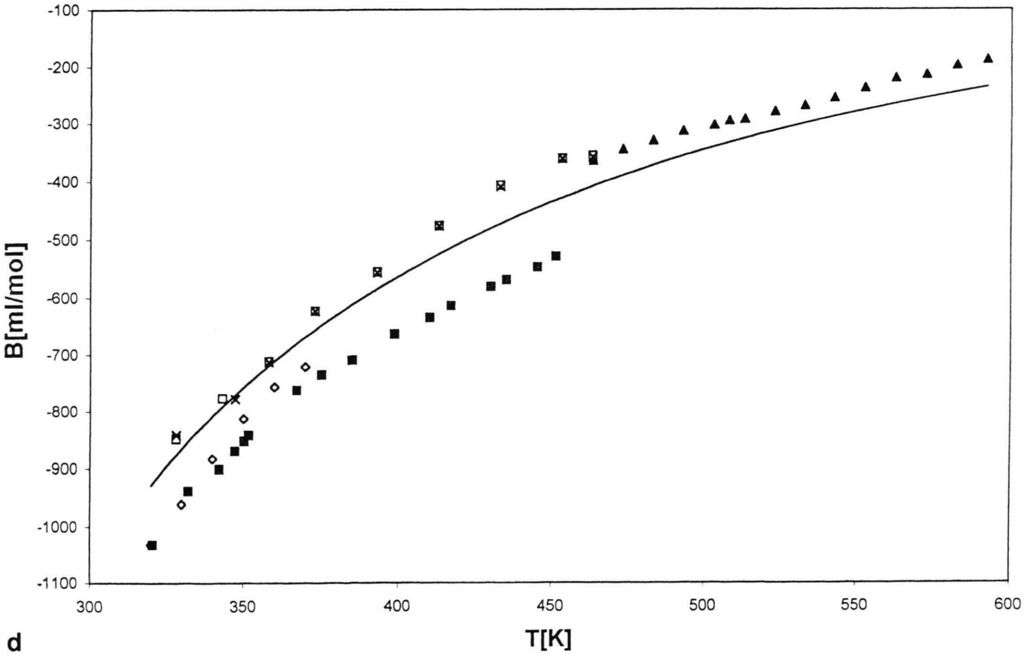

-100
-200
-300
-400
-500
-600
-700
-800
-900
-1000
-1100
B[ml/mol]
300
350
400
450
500
550
600
T[K]
d

Fig. 2 c, d

Table 4. The ε/k and σ parameters of uranium hexafluoride for different potentials.

Potentials	ε/k [K]	σ [Å]	n	Ref.
Lennard-Jones $(6, n)$ potential	224	8.3	$n=12$	[17]
	258 ± 6	7.1 ± 0.06	$n=12$	[18]
	430	5.24	$n=12$	[19]
	399.8	6.5 ± 0.5	$n=12$	[20]
	617.1	5.3	$n=13.58$	[12]
Kihara potential	1140 ± 90	1.8 ± 0.2		[21]
Modified (exp-six) Buckingham potential	582	5.44	$\alpha=14.75$	[22] [23] [24]
Aziz MMSV potential	764 ± 2	5.01 ± 0.1		This paper

Brown [30] 1.2–2.7%; the thermal conductivity data, Schimid [22] 2.5–4.1% and De Witt [27] 1.1–1.8%. For the second virial coefficient data we have the following deviations: Malyshev [17] 6–11 ml/mol, Malyshev [18] 11–20 ml/mol, Morizot [13, 19] 0.5–13 ml/mol, Heintz [12] 10–23 ml/mol, which correspond to the 0.1–3.5% percentage deviations with the exception of high temperature Malyshev determinations [18], above 550 K, where these are 5–8%.

In Fig. 2, we have represented the temperature dependence of the experimental and calculated data with the MMSV potential for the viscosity, thermal conductivity, self-diffusion and virial coefficient.

Although, we have used all the presently available literature data, and of course these data present some scatter, the Morse-Morse-Spline-van der Waals (MMSV) potential can provided an excellent overall reproduction of both transport properties and virial data at the same time. Clearly, the MMSV potential [5], of all those previously considered [12, 17–24], has the best overall predictive ability for uranium hexafluoride data.

5. Conclusions

We present numerical values of the reduced second virial coefficients, reduced collision integrals and higher approximations to the transport coefficients for the MMSV potential over a large reduced temperature range, kT/ε from 0.1 to 100. These results can be used to characterize the bulk properties of various spherical molecules, especially to predict gaseous transport properties.

Also, we present the potential parameters of uranium hexafluoride established by us for the MMSV potential, together with the potential parameters determined previously, for Lennard-Jones [12, 17–20], Kihara [21] and modified (exp-six) Buckingham [22–24] potentials.

For uranium hexafluoride, the Morse-Morse-Spline-van der Walls potential [5] predicts the best viscosity, thermal conductivity, self-diffusion and second virial data, simultaneously, in a manner better than any other literature potential.

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