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Pair Interaction Potential Energy Function from the Extended Principle of Corresponding States for SF_6-SF_6

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An iterative inversion procedure is used to obtain the effective isotropic part of the pair-interaction potential for SF_6-SF_6 from the extended principle of corresponding states. The Lennard-Jones (12-6) potential energy function is used as the initial model potential required by the method. Over a range of reduced temperature extending from 1 to 1000 this directly measured potential for SF_6-SF_6 fully agrees with the Hartree-Fock-Dispersion (HFD)-type and Morse-Morse-Spline-vander Waals (MMSV)-type independently known potentials. This accurate inverted potential can be used in the calculation of the orientation-averaged viscosity collision integrals and the dimensionless ratios which are essential to calculate other transport properties. Our method can be applied to calculate the pair-interaction potential with no need for force fitting data and lengthy multi-parameter fitting procedure in all temperature ranges.

Key Words: Interaction potential, Collision integrals, Direct inversion method, Extended principle of corresponding states.

INTRODUCTION

For as long as the idea of atoms and molecules has existed man has speculated as to the nature of the forces between them. The Greek and Roman atomist philosophers saw the forces in concrete terms and hence, people used to think strongly interacting molecules as "hooked and intertangled". Many observable properties of matter depend upon pairwise intermolecular potential energy function. The results of kinetic and statistical-mechanical theories provide theoretical expression for various equilibrium and non-equilibrium properties in terms of the potential energy of interaction between a pair of molecules[1–4], therefore, the evaluation of such quantities from a known pair-potential energy function is not especially difficult. However, the inverse operation is not generally straight forward.

Intermolecular forces are responsible for many of the bulk properties of matter; for example, a realistic description of the relationship among pressure, volume and temperature of a gas must include the effects of attractive and repulsive forces

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between molecules. Accurate knowledge of the pair-potential energy functions is essential in order to obtain quantitatively information on many body forces in a system. The importance of intermolecular forces has been responsible for their extensive study for many decades.

Knowledge of the intermolecular potentials opens the way to the calculation of many observable properties, for microscopic as well as macroscopic systems. In the first category are the spectra of van der Waals molecule[5, 6] and molecular beam scattering cross-section[7, 8], elastic or inelastic state-to-state, total or differential properties[9,10]. In the second category are various bulk gas and condensed matter properties. Measured gas phase properties that depend directly on the intermolecular potential are: virial coefficients; viscosity and diffusion coefficients and thermal conductivity[11–13].

A knowledge of the forces between molecules is fundamental to an understanding of the structure and properties of physical and biological materials. There are a number of elementary papers[14–18] concerned with the methodology of the direct inversion procedure; these reasonably give more than superficial attention to a consideration of molecular interactions. In recent years, considerable advances have taken place in the field of intermolecular forces and it is now possible to give a definitive account of the interactions between many of the simplest molecules; at the same time the routes to understanding more complex systems have become easier[19–24]. At this level, a far wider range of systems may be considered by several authors.

Precise determination of the forces between atoms and molecules remains one of the most important prototypical problems in molecular physics. Determination of the intermolecular forces from a macroscopic property has the following restrictive condition: (i) It has to be experimentally measurable with sufficient accuracy. (ii) It is necessary that there exist a refined theoretical description of the property.

The relationship between such properties and the forces that exist between molecules is important because it forms the basis of many of the methods used to correlate and predict thermophysical properties; these provide the means to reduce the amount of experimentation required to a manageable level. The same relationship allows information to be gained about intermolecular potential from the study of the properties of gases. If we can obtain such information from one property then we may be able to calculate another useful property of gas, at any temperature, and thereby relieve ourselves of the need to measure it.

However, there exists a great deal of interest in the scientific community for obtaining the intermolecular potential energy function to be used in the prediction of equilibrium and transport properties of gases.

The traditional approach which has a long history for the determination of neutral-neutral interaction potentials from macroscopic properties is the use of a mathematical model potential containing a few parameters and adjusting these parameters such that agreements between theoretical and experimental properties of matter is obtained. But for example the parameters determined from the equilibrium properties (second virial coefficients and Joule-Thomson coefficient) are slightly different from those determined from non-equlibrium properties (viscosity and self-diffusion).

For these reasons, one of the central objectives of chemical physics of gases has been and remains the expression of bulk thermophysical properties in terms of molecular quantities. In such a description, chemical physicist seek to relate characteristics of the bulk gas, such as viscosity, to the properties of individual molecules that make up the gas and the intermolecular potential that exists between them[1–4, 11–13].

A very precise extended principle of corresponding states has been formulated for the noble gases and eleven polyatomic gases at low density[25, 26]. It has been proved that it is capable of correlating equilibrium and transport properties of noble gases, eleven polyatomic gases and their multi-component mixture, over a wide temperature range, with an accuracy commensurate to the best measurements[27]. The principle seeks the maximum use of theory and experiment that can be obtained without assumptions about the functional form of the pair interaction potential.

Of particular value is the development of an inversion technique for bulk properties, which are readily available for a wide variety of substances. The inversion scheme is an important method for generating the intermolecular potentials from the bulk properties and their corresponding state correlation. Among the bulk properties, transport properties and especially viscosity are among the important sources for the extraction of information about the intermolecular potential energy.

One can ask two questions about any set of measurements of a bulk property:

(i) What specific information about pair-interaction does it contain?

(ii) How can the information be extracted directly?

The inversion technique yields reliable answers to the aforesaid questions[15–24, 28–32]. The first inversion of viscosity data was due to Dymond[33] who used a method based on one devised by Hirschfelder and Eliason[34] for calculating approximate transport properties economically.

We believe that the direct inversion method should serve a dual purpose: (1) to illustrate and test theoretical principles of kinetic theory of gases; and (2) to reproduce the reduced collision integrals and their dimensionless ratios, which are necessary and sufficient information to obtain transport properties of gases.

On the other hand, severe limitations of time and equipment must be faced in providing a set of experiments that produce physical measurements that yield quantitative results in a reasonably broad coverage of wide and varied topics of transport properties of gases.

Meanwhile direct inversion procedures for the potential energy functions of noble gases and mixtures of polyatomic gases with nobel gases from data on viscosity have been re-examined by Najafi *et al.*,[35–39] and others[40, 41] in connection with the extended principle of corresponding states[27].

It should be mentioned that there is large literature dealing with SF_6 giving an overwhelming amount of information[42, 43] some of which is vital for representing effective isotropic pair interaction potential of SF_6.[44]

In this paper we present an interaction potential energy function for sulfur hexafluoride (near-spherical) molecules which were calculated by using the inversion method based on the experimental reduced collision integral obtained from corresponding-states correlation[27]. By a near-spherical molecule we mean a molecule which has a number of similar atoms symmetrically distributed over the surface of a sphere whose centre may or may not be occupied by another atom. Because of its high degree of symmetry and lack of dipole moments it is reasonable to base a theoretical treatment of an assembly of near-spherical molecules on the assumption that the force between any pair of molecules depends upon their separation but not upon their orientation. Hence, spatially-oriented internal degrees of freedom are ignored. Comparison of these results with the HFD-type independently known potential of Mienander[44] shows good agreement and clearly adequate.

Collision Integral

Once the interaction potential is known, transport properties can be obtained from the Chapman-Enskog solution of the integrodifferential Boltzmann-kinetic equation, the transport properties (viscosity, thermal conductivity, diffusion coefficients and thermal diffusion factor) can all be calculated if the reduced collision integrals, $\Omega^{(l,\,S)*}$, are known. These collision integrals are Boltzmann factors of transport cross sections, $Q^{(1)*}$, and defined in the standard source book[12].

The collision integrals, which carry the information of the two-body interaction, are also therefore functions of the intermolecular potential between any two given particles[11–13]. In the present work, the two-body interaction will be taken to be between particles.

The collision integral $\Omega^{(l,\,S)*}$ is the first of a family of consecutive integrals that arise in the kinetic theory derivations[11–13].

$$\Omega^{(l,\,s)*} = [(s+1)!\,(kT)^{s+2}]^{-1} \int_0^\infty Q^{(l)}(E)\, e^{-E/kT}\, E^{s+1}\, dE \tag{1}$$

where E is the relative energy of colliding partner, and $Q^{(l)}(E)$ is a transport cross section that classically is given by the equation:

$$Q^{(l)}(E) = 2\pi\{1 - [1 + (-1)^l/2(l+1)]\}^{-1} \int_0^\infty (1 - \cos^l \theta) b\, db \tag{2}$$

in which θ is the relative deflection angle between two colliding partners of energy E and impact parameter b at the gas temperature.

The deflection angle θ is calculated as a function of b and E from the classical equation of motion.

$$\theta(b, E) = \pi - 2b \int_{r_0}^\infty [1 - b^2/r^2 - V(r)/E]^{-1/2}\, dr/r^2 \tag{3}$$

where the distance of closest approach r_0 is the outermost root of

$$1 - b^2/r_0^2 - V(r_0)/E = 0 \tag{4}$$

Numerical differentiation and use of the recursion relation can generate collision integrals higher than that mentioned,

$$\Omega^{*(l,\,s+1)} = \Omega^{*(l,\,s)}\left[1 + \frac{1}{s+2}\,\frac{d\ln\Omega^{*(l,\,s)}}{d\ln T^{*}}\right] \tag{5}$$

where the reduced collision integral is defined by

$$\Omega^{*(l,\,s)} = \frac{\Omega^{(l,\,s)}}{\pi\sigma^{2}} \tag{6}$$

where σ is length scaling factor such that $V(\sigma) = 0$. Reduced temperature (T^*) is defined as

$$T^{*} = kT/\varepsilon \tag{7}$$

ε is energy scaling factor.

Inversion Method

The existence of the refined theoretical description of transport properties is necessary condition—to within our information—for determination of the forces between atoms and molecules. Because of the aforesaid restriction, most of our knowledge has been obtained from properties of dilute gases. By dilute, we mean that the rates of transport of mass, momentum and energy are controlled by binary molecular collision. In other words, it means densities sufficiently low that only two-body collisions need be considered.

The kinetic theory of gases yields theoretical expressions for the viscosity, thermal conductivity and other transport properties of gases and the results are in reasonably good agreement with experiment. The rigorous kinetic theory treatment of transport properties in gases is extremely complicated mathematically and physically. The rigorous expressios underlying transport phenomena in gases were worked out in 1860 and 1870 by Maxwell and Boltzmann, but it was not until 1917 that Sydney Chapman and David Enskog, working out independently, solved the equations[45].

For a dilute gas the viscosity as given by the rigorous expression for the viscosity, η, of a dilute gas by the Chapman-Enskog solution of Boltzmann equation is[12]

$$\eta(T) = \frac{5}{16\sigma^{2}}\,\frac{(mk_{B}T/\pi)^{1/2}}{\langle\Omega^{(2,\,2)*}\rangle}\,f_{\eta} \tag{8}$$

where m is the molecular mass, k_B is the Boltzmann constant, and f_η is a "second order Kihara" correction factor for the calculation of transport properties which normally differs from unity by only 1 per cent. We have set the value of f_η equal to unity.

$\langle\Omega^{(2,\,2)*}\rangle$ is orientation-averaged reduced viscosity collision integral which is defined in general form as:

$$\langle\Omega^{(2,\,2)*}\rangle = \frac{1}{\pi}\int_{0}^{\pi}\int_{0}^{1}\int_{0}^{1}\Omega^{(2,\,2)*}\,d\phi\,d(\cos\theta_{1})\,d(\cos\theta_{2}) \tag{9}$$

where $\langle \Omega^{(2,2)*} \rangle$ is orientation-averaged reduced viscosity collision integral. Writing the collision integrals in the form of eq (9) is tantamount, by the way, to assuming that the post-averaging approximation has been used throughout the entire temperature range. The transport properties were calculated using Monchick-Mason approximation which provides a simple scheme whereby the collision integrals may be calculated. The principal assumptions made in their approach are first, the energy transfer between translation and internal modes does not affect the transport properties and, second, the relative angular orientation of the molecules remains unchanged throughout the collision process. They suggested therefore that the calculation should be performed by computing the fixed angle collision integrals $\Omega^{(l,s)}(T, \phi, \theta_1, \theta_2)$ for the collision of two molecules at the fixed relative orientation. The collision integral for the effective isotropic potential is then obtained quite simply by averaging the fixed orientation collision integrals with equal weight over all space (as mentioned in Eq (9)).

Strictly speaking, the Chapman-Enskog kinetic theory of gases applies only to monatomic gases (molecules with no internal degrees of freedom for which the interaction potential is spherically symmetric). Inelastic collisions occur between molecules with internal degrees of freedom. In these collisions kinetic energy is no longer conserved, albeit clearly mass and momentum are conserved. Consequently, the viscosity and diffusion are not appreciably affected by the presence of the internal degree of freedom, and the theory of monoatomic gases may be applied to polyatomic molecules with considerable success. On the other hand,viscosity and diffusion involve, respectively, moment and mass transfer, they should not be affected significantly in the first approximation by internal degrees of freedom and hence can serve as one of the best sources of information for the intermolecular forces in polyatomic gases.The viscosity coefficients of polyatomic gases are correlated in the extended principle of corresponding states[27] by the equation:

$$\langle \Omega^{(2,2)*} \rangle = \exp [0.46641 - 0.56991 (\ln T^*) + 0.19591 (\ln T^*)^2 - 0.03879 (\ln T^*)^3 + 0.00259 (\ln T^*)^4], \; 1 \leq T^* \leq 10 \qquad (10a)$$

$$\langle \Omega^{*(2,2)} \rangle = (\rho^* \alpha)^2 [1.04 + a_1 (\ln T)^{-1} + a_2 (\ln T^*)^{-2} + a_3 (\ln T^*)^{-3} + a_4 (\ln T^*)^{-4}] \; 10 \leq T^* \leq 100 \qquad (10b)$$

in which $\langle \Omega^{(2,2)*} \rangle$ and T^* are defined by the eqns. (6, 7). The values of ρ^* and V_0^* (adopted from ref. 27) are given in Table 3.

The values of a's are given as follows:

$a1 = 0$

$a2 = -33.0838 + (\alpha_{10} \rho^*)^{-2} [20.0862 + (72.1059/\alpha_{10}) + (8.27648/\alpha_{10})^2]$

$a3 = 101.5710 - (\alpha_{10} \rho^*)^{-2} [56.4472 + (286.3930/\alpha_{10}) + (17.7610/\alpha_{10})^2]$

$a4 = -87.7036 + (\alpha_{10} \rho^*)^{-2} [46.3130 + (277.1460/\alpha_{10}) + (19.0573/\alpha_{10})^2] \qquad (11)$

In the aforesaid relations $\alpha_{10} = \ln (V_0^*/10)$ is the value of $\alpha = \ln (V_0^*/T^*)$ at the matching point of T* = 10. No one has yet figured out the correlation formula for the reduced collision integrals for the polyatomic gases in low temperature region ($T^* < 1$). The expression of $\langle \Omega^{*(2,2)} \rangle$ in the low temperature region ($T^* < 1$) has not been obtained, since (i) the experimental information of viscosity at low temperatures is not available and (ii) the existence of several long-range contributions to the interaction potential whose effects on the low-temperature properties can neither be calculated nor separated.

The inversion technique initiates by estimation of G_η, inversion function, from an initial model potential such as LJ (12-6). The inversion function is a function of the reduced temperature(T*) alone[14]. We have estimated this function using LJ (12-6) model as the initial model[46].

Given a set of reduced viscosity coefficient collision integrals, $\langle \Omega^{*(2,2)} \rangle, T^*))$ over a wide range of reduced temperature from the extended law of corresponding states on the one hand, and estimating the G_η function from initial model potential LJ (12-6) on the other, it is possible to transform a pair of datum $((\langle \Omega^{*(2,2)} \rangle, T^*)$ to V/ε versus r/σ on the potential energy curve and hence we can marshal two steps of inversion procedure:

$$V/\varepsilon = V^* = G_\eta(T^*)T^* \tag{12}$$

$$r/\sigma = r^* = (\Omega^{*(2,2)})^{1/2} \tag{13}$$

Equations (12) and (13) are central equations in the inversion scheme.

The new potential is a closer approximation to the true potential energy than the potential of the initial model. The new $G_\eta(T^*)$ can be obtained from square interpolation among new potentials. These new potentials have been used to calculate improved collision integrals. Numerical integrations have been carried out for the evaluation of the integral equations (1–3) with these new potentials. The above process is repeated until convergence occurs. The convergence criteria are judged by: (i) the extent to which the calculated collision integrals are in accordance with the reduced viscosity coefficient collision integrals determined by the extended law of corresponding states, eq. (10a–10b).In this work, the three consecutive integrals are evaluated to within an accuracy of 0.1%. This accuracy is obtained by comparing the calculated values of collision integrals with the experimental ones in each iteration. (ii) the degree to which the intermolecular potential energies obtained by inversion method reproduce thermophysical properties within the experimental accuracy. (iii) the degree to which the potentials are unchanged from one iteration to the next. It should be said that the rate of convergence of iterations reflects the differences of detail between the initial model $V_0^*(r^*)$ and true model $V^*(r^*)$. Our results converged after two iterations and the results are given in the next section.

RESULTS AND DISCUSSION

We have used our reasonably effective isotropic potential to obtain the improved collision integrals necessary for the calculation of transport proerties. Collision integrals in conjunction with their ratios are shown in Table-1. The ratios of collision integrals have been calculated by the following equations[12]

$$A^* \equiv \frac{\langle \Omega^{(2,2)*} \rangle}{\langle \Omega^{(1,1)*} \rangle}, \quad (14)$$

$$B^* \equiv \frac{5\langle \Omega^{(1,2)*} \rangle - 4\langle \Omega^{(1,3)*} \rangle}{\langle \Omega^{(1,1)*} \rangle}, \quad (15)$$

$$C^* \equiv \frac{\langle \Omega^{(1,2)*} \rangle}{\langle \Omega^{(1,1)*} \rangle}, \quad (16)$$

$$E^* \equiv \frac{\langle \Omega^{(2,3)*} \rangle}{\langle \Omega^{(2,2)*} \rangle}, \quad (17)$$

$$F^* \equiv \frac{\langle \Omega^{(3,3)*} \rangle}{\langle \Omega^{(1,1)*} \rangle}. \quad (18)$$

TABLE-1.
DIMENSIONLESS COLLISION INTEGRALS AND RELATED RATIOS FOR SF_6-SF_6

$\log_{10} T^*$	$\langle \Omega^{(2,2)*} \rangle$	A*	B*	C*	E*	F*
0.0	1.57369	1.12263	1.21019	0.85644	0.88471	0.93161
0.1	1.41750	1.11452	1.17874	0.86288	0.88941	0.93401
0.2	1.28568	1.10739	1.15163	0.87371	0.89925	0.94063
0.3	1.17817	1.10244	1.13036	0.88665	0.91127	0.95032
0.4	1.09174	1.09973	1.11448	0.89984	0.92311	0.96154
0.5	1.02210	1.09863	1.10282	0.91206	0.93347	0.97278
0.6	0.96524	1.09835	1.09417	0.92272	0.94194	0.98296
0.7	0.91794	1.09832	1.08766	0.93165	0.94870	0.99150
0.8	0.87785	1.09830	1.08290	0.93892	0.95416	0.99818
0.9	0.84339	1.09840	1.07994	0.94464	0.95875	1.00305
1.0	0.81344	1.09900	1.07879	0.94892	0.96260	1.00650
1.1	0.78698	1.10024	1.07855	0.95192	0.96533	1.00941
1.2	0.76270	1.10147	1.07710	0.95407	0.96629	1.01273
1.3	0.73916	1.10115	1.07216	0.95612	0.96536	1.01682
1.4	0.71534	1.09750	1.06273	0.95888	0.96347	1.02099
1.5	0.69118	1.08958	1.04974	0.96289	0.96215	1.02404
1.6	0.66755	1.07777	1.03534	0.96820	0.96270	1.02505
1.7	0.64577	1.06354	1.02180	0.97434	0.96564	1.02388
1.8	0.62701	1.04882	1.01061	0.98068	0.97063	1.02113
1.9	0.61197	1.03328	1.00235	0.98658	0.97677	1.01767
2.0	0.60078	1.02397	0.99691	0.99162	0.98308	1.01423

Our effort was just devoted to the calculations for which $T^* > 1.0$. The reason for this may be stated thus: No one has yet figured out the correlation formula for the reduced collision integrals for the polyatomic gases in low temperature regime ($T^* < 1.0$). Hence, we do not have any relation for inversion (such as eq.

(11)) in this region. Consequently, in order to integrate eqs. (1–3) over the given range it is necessary to extrapolate V(r) in the long range region (low temperature). The extrapolating function which we used was $V^* = -C_6u^6$, where C_6 is the dispersion coefficient and u is the reciprocal of the intermolecular distance (both in atomic units). C_6 has been estimated from the latest datum point in the attractive region.

Regarding the aforesaid discussion and existence of corresponding states viscosity coefficients at high temperatures (repulsive region) the inversion was established. It should be mentioned that albeit we used just $V^* = -C_6u^6$ as extrapolating function at long range region, the inversion function procedure is not unduly sensitive to the nature of the used extrapolating functions. This is due to the fact that the potential will adjust itself during iteration steps. As mentioned before, the inversion function $G_\eta(T^*)$ is found to be remarkably insensitive to the precise nature of the potential, a feature which greatly enhances the convergence rate of the inversion. It is worthwhile to be noted that for a given transport property, G(T) is determined by the ratio of the impact parameter to the distance of closest approach for a collision at an energy $\cong (s + 1)kT$ which results in a deflection angle of $\theta \sim \pi^{-1}$.[19] It is remarkable to mention that in order to maintain this deflection angle constant as the potential changes, requires the impact parameter to be changed; the distance of closest approach will change in the same direction and by roughly the same magnitude due to this small deflection angle, the impact parameter and the distance of closest approach are similar. One therefore expects their ratios, and hence the G(T) function (and consequently extrapolating function), to be essentialy independent of the precise nature of the potential.

We chose the HFD-type potential model as the reference system as shown in Fig. 1. The precise value of $\varepsilon/\varepsilon_{ref}$ is 0.98531 for SF_6-SF_6. The reason for giving precise values of these parameters is that it should be sufficient to determine many properties of gaseous mixtures, because of the existence of a successful limited principle of corresponding states for low density molecular gases[26], in which the parameters σ and ε are used as scale factors of energy and molecular size for the correlation and prediction of both equilibrium and transport properties[27]. The values of the dimensioned scaling potential parameters obtained in this work are given in Table-2. Comparison of this result with the HFD-type independently known potential, Mienander[44] shows a good agreement and clearly adequate. It is worthwhile to be noted that the value of σ turns out to be equal to the value of σ_0 such that $V(\sigma_0) = 0$; the precise values of σ/σ_0 is 0.99614. The result obtained here covers the range from the potential-energy minimum inwards to a repulsion of the well depth. In this work, the potential well depth could be obtained as the relative value with respect to a convenient reference system. Since

TABLE-2

DIMENSION OF SCALING PARAMETERS σ AND ε/k_B FOR SF_6-SF_6

	σ (Å)	ε/k (K)
SF_6-SF_6	5.2317	339.69

the HFD potential[45] used was generated on a sound experimental basis, the selection of it as reference system is quite reasonable.

As shown in Figs. 1 and 2, the viscosity data provide us only the potentials at distances $r \leq \sigma$. On the other hand, it can be shown that the width of the potential energy function is related to the second virial coefficient, B, with the equations[15]

$$V^* = T^* - 1 \tag{19}$$

and

$$r_R^{*3} - r_L^{*3} = -2\pi N_0/3(B^* - 1)N(T^*) \tag{20}$$

where r_R^* and r_L^* are the reduced coordinates of the outer and inner wall of the potential well, respectively. The quantity N_0 is Avogadro's number, $N(T^*)$ is the second virial inversion function tabulated in ref. [15], and $B^* = 3B/2\pi N_0\sigma^3$ is the reduced second virial coefficient. Knowing the inner branch of the potential well from the viscosity, we can use this information in conjunction with the second virial coefficient data to determine the outer branch of the well uniquely (as shown in Figs. 1 and 2).

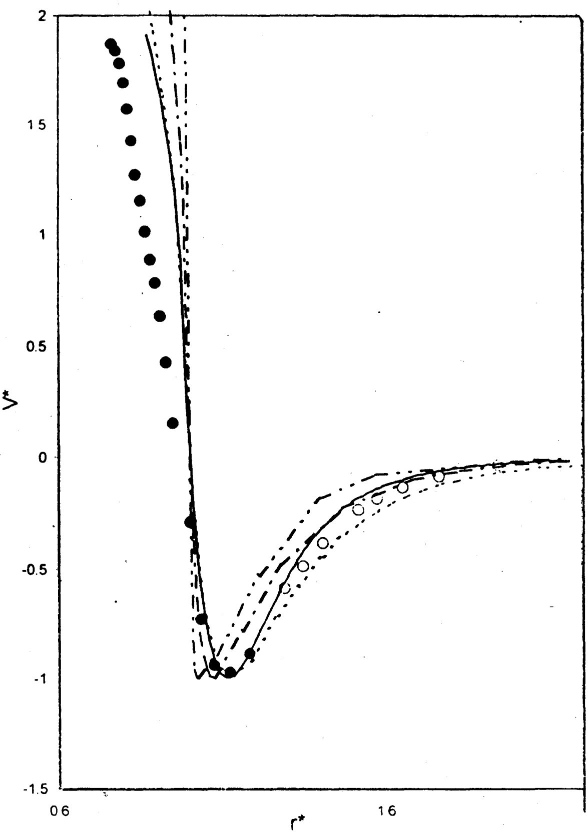

Fig. 1. Reduced pair interaction potential for SF_6-SF_6. (•) results obtained by the corresponding-states viscosity and (o) second virial, (—) the HFD-type potential (model c of ref. [44]), (– – –) the HFD-type potential (model f of ref. [44]), (– · · · – · ·) the MMSV-type potential [ref. 49] and (........) the LJ(12-6)-type potential[48].

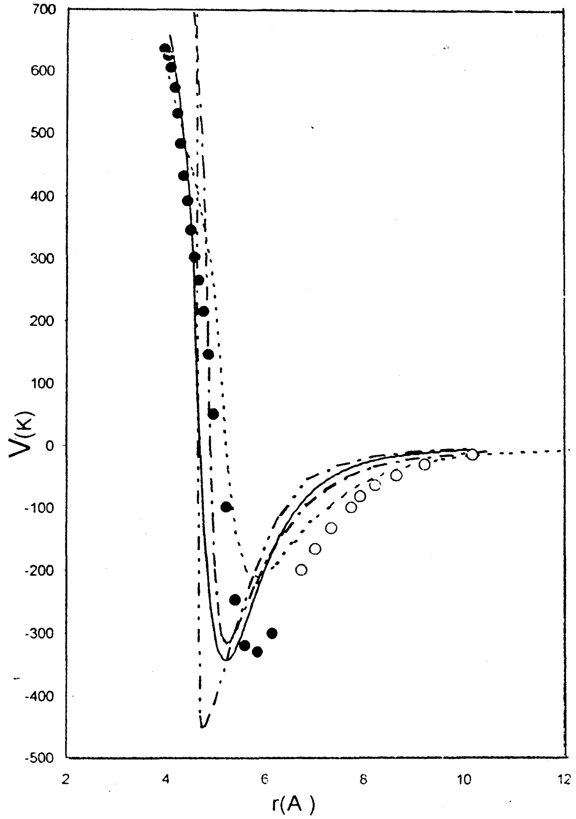

Fig. 2. Pair interaction potential for SF_6-SF_6. The symbols are same as in Fig. 1.

TABLE-3
LOW AND HIGH TEMPERATURE DIMENSIONLESS SCALING PARAMETERS (Taken from ref. [27]).

	ρ^*	V_0^*
SF_6–SF_6	0.050	4.067×10^8

A conclusion central to our study is that it seems to describe an interesting example of the application of the direct inversion method to calculate the intermolecular potential energy curve for an important prototypical system. The inverted potential can be used to obtain reduced collision integrals and their dimensionless ratios which are needed to calculate other transport properties. This can be obtained with more accuracy than is possible by a corresponding-state analysis of such properties, primarily because viscosity measurements are more accurate than measurements of other properties.

It should also be mentioned that we could observe some discrepancies between the potential energy obtained from the inversion method, that we have claimed to be reliable and the potential energy function depicted in Fig 1. These discrepancies are explicitly seen in the short-range region. It is worthwhile to be noted that the revision of the extended principle of the corresponding states by Najafi *et al.*[25] and Bzowski *et al.*[27] correlates properties of the noble gases, molecular gases and all their mixtures at low density regime over a very large temperature range with excellent accuracy and characterizes each binary interaction with the aid of five parameters, *i.e.*, σ, ε, V_0^*, ρ^*, C_6^*. C_6^* characterizes well the long-range attractive tail of potential ρ^* and V_0^* characterizes the short-range repulsive one. Since the later parameter was rigorously generated on a sound experimental basis, so the pair-interaction potential obtained *via* inversion method is highly reliable.

Calculations of other properties are considerably eased by introducing Table-1. In this work, the three consecutive integrals are evaluated using the computer program developed by O'Hara and Smith[47]. Therefore, toward the eventual goal of a fundamental and unambiguous methodology of the inversion procedure, the objective of the present paper is to understand that the application of the aforesaid method appears to be quite reasonable.

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