is fulfilled are arranged in the form of an increasing sequence of q: q = 1, 2, ..., Q. Then the sought value of $p_\theta(n, \hat{x})$ is determined by the expression

$$p_\theta(n, \hat{x}) = \sum_{q=1}^{Q} y(s_q) - \sum_{q=1}^{Q-1} y(s_q + 1) - y(1), \tag{17}$$

in the same way with the aid of formula (6) we find the parallel projection, and with a view to formulas (2), (3) we find the bundle projection for any image $\mu(x, y)$ from among the class under examination.

NOTATION

x, y, Cartesian coordinates; i, imaginary unit; r, φ, polar coordinates; $w = x + iy = r\exp(i\varphi)$; $\hat{w} = \hat{x} + i\hat{y} = w\exp(-i\theta)$; $\mu(x, y)$, absorption coefficient of radiation as a function of the coordinates (image of the section of the object); β, γ, bundle coordinates; $p_\theta(\hat{x})$, parallel tomographic projection; $h_\beta(\gamma)$, bundle tomographic projection.

LITERATURE CITED

1. H. J. Scudder, "Introduction to computer aided tomography," Proc. IEEE, 66, No. 6, 628-637 (1978).

SURVEYS

INTERACTIONS OF ATOMS AND CALCULATION OF TRANSPORT COEFFICIENTS IN METAL VAPORS AND THEIR MIXTURES WITH GASES

K. M. Aref'ev and M. A. Guseva

UDC 533.15

In kinetic theory [1, 2], the transport coefficients of a gas are expressed in terms of collision integrals. In particular, in the first approximation of the theory of Chapman and Enskog, the viscosity and thermal conductivity of a dilute, single-component gas, and the coefficient of diffusion of a dilute binary mixture are given by the formula

$$\eta = \frac{5}{16}\,\frac{\sqrt{\pi m k T}}{\pi\sigma^2\Omega^{(2,2)*}}, \tag{1}$$

$$\lambda = \frac{5}{2}\,\eta c_v \tag{2}$$

(for a monatomic gas),

$$D_{12} = \frac{3}{16 n m_{12}}\,\frac{\sqrt{2\pi m_{12} k T}}{\pi\sigma_{12}^2\,\Omega_{12}^{(1,1)*}}. \tag{3}$$

The reduced collision integrals

$$\Omega^{(l,s)*} = \Omega^{(l,s)}\left\{\left(\frac{kT}{\pi m_{12}}\right)^{1/2}\frac{(s+1)!}{2}\left[1 - \frac{1+(-1)^l}{2(l+1)}\right]\pi\sigma_{12}^2\right\}^{-1}$$

are computed with the help of relations taking into account the interaction of molecules in collisions based on the conservation laws of mass, momentum, and kinetic energy:

$$\chi(g, b) = \pi - 2b\int_{R_m}^{\infty}\frac{dR/R^2}{[1 - b^2/R^2 - \varphi(R)/(m_{12}g^2/2)]^{1/2}},$$

M. I. Kalinin Polytechnical Institute, Leningrad. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 50, No. 1, pp. 148-162, January, 1986. Original article submitted November 16, 1984.

0022-0841/86/5001-0109$12.50

$$Q^{(l)}(g) = 2\pi \int\limits_0^\infty (1-\cos^l\chi)\, b\,db,$$

$$\Omega^{(l,s)} = \sqrt{kT/(2\pi m_{12})} \int\limits_0^\infty \exp(-\gamma^2)\, \gamma^{2s+3}\, Q^{(l)}(g)\, d\gamma,$$

where

$$\gamma = g\,(2kT/m_{12})^{1/2}\,.$$

When $R = R_m$, the denominator of the integrand in the expression for χ goes to zero and the contribution of the kinetic energy $m_{12}g^2/2$ is comparable to that of the effective potential energy $(m_{12}g^2/2)(b^2/R^2) + \varphi(R)$, and this defines an equation for R_m. The collision integrals $\Omega^{(l,s)}$ have the dimensions of velocity multiplied by the square of a linear dimension (area) and average the cross section $Q^{(l)}$ over the relative molecular velocities γ with weight s. Both $\Omega^{(l,s)}$ and the dimensionless reduced collision integrals $\Omega^{(l,s)*}$ depend on the interaction potential energy of the molecules $\varphi(R)$.

In the usual method of calculating the transport coefficients, the Lennard–Jones or Buckingham potentials [1, 2] or the Monchick potential [3], are used for $\varphi(R)$, and the integrals $\Omega^{(l,s)*}$ have been tabulated for several potentials as functions of the parameters. For example, in the Lennard–Jones potential

$$\varphi(R) = 4\varepsilon\,[(\sigma/R)^{12} - (\sigma/R)^6] \qquad (4)$$

the integrals $\Omega^{(l,s)*}$ are given as functions of $T^* = kT/\varepsilon$. The parameters of the model potentials (σ and ε in the case of the Lennard–Jones potential) are found in the case of pure gases from experimental data on the viscosity (with the use of the formula given above for η from kinetic theory) and also can be estimated from the molar volumes of the solid or liquid phases, the critical molar volume, the melting and boiling temperatures, and the critical temperature. It is also possible to determine the potential parameters from the second virial coefficient of the equation of state. The parameters for binary mixtures are found in terms of the parameters of the components on the basis of the combination rule approximation. For the Lennard–Jones potential

$$\sigma_{12} = (\sigma_1 + \sigma_2)/2, \quad \varepsilon_{12} = \sqrt{\varepsilon_1\varepsilon_2} \qquad (5)$$

and the second formula applies only for molecules with nearly the same ionization energies [1].

It is possible to theoretically determine the interaction potential energy for identical and for different molecules (most simply for monatomic molecules)* with the help of quantum-mechanical methods. Such calculations are particularly important since, for example, in the calculation of the transport coefficients in mixtures of alkali metal vapors with inert gases, application of the combination rules leads (in principle) to incorrect results because the parameters of the model potentials for pure alkali metal vapors are only effective parameters [4-6]. They take into account the contribution of triplet (same spin orientation of the valence electrons of the atoms) and singlet (opposite spin orientation) interactions between the alkali metal atoms.† The total collision integral (cross section) is obtained by summing the integrals corresponding to the triplet (with weight 3/4) and singlet (with weight 1/4) interactions; but the interaction of metal atoms with inert gas atoms (with two or more electrons in the outer shell with pairwise opposite spins) is different in nature and splitting of the terms does not occur.

Quantum-mechanical calculations of the pair interaction potential energy of molecules (or atoms in the simpler case of monatomic gases considered below) is based on the solution of the Schrödinger equation in the Born–Oppenheimer approximation of fixed (frozen) nuclei for the electron wave function $\Psi(R, r)$ [7-10]:

---

*Inert gases and hot metal vapors are obviously monatomic (impurities of diatomic molecules are insignificant).

†Examples are the interactions of two hydrogen atoms or the interaction between an alkali metal atom and a hydrogen atom.

$$\hat{H}_e \Psi(R, r) = E(R)\,\Psi(R, r), \tag{6}$$

where r is the set of electron coordinates, E is the interaction energy of the electrons moving in the field of the nuclei, and the interaction energy of the nuclei.

The Hamiltonian $\hat{H}_e$ takes into account the kinetic energy of the electrons, the energy of attraction of the electrons to the nuclei, the energy of repulsion of the electrons and the energy of repulsion of the nuclei. In atomic units (a.e.) where $m_e = e = \hbar = 1$:

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_i \left(\frac{Z_a}{r_{ia}} + \frac{Z_b}{r_{ib}}\right) + \sum_{i<j} \frac{1}{r_{ij}} + \frac{Z_a Z_b}{R},$$

where ∇_i^2 is the Laplacian with respect to the electron coordinates; Z_a and Z_b, nuclear charges of the interacting atoms a and b; r_{ia} and r_{ib}, distances between the i-th electron (since we are treating the electrons of both atoms) and the nucleus a or b; and r_{ij}, distance between the i-th and j-th electrons.

The quantity E(R) obtained from the solution of the Schrödinger equation (6) determines the interaction potential energy of the atoms at distance R (the adiabatic potential):

$$\varphi(R) = E(R) - E(\infty), \tag{7}$$

where $E(\infty) = E_a + E_b$ is the total energy of the atoms at infinite separation.

Since the mass of the nucleus of any atom is much larger than the mass of the electron, the Born–Oppenheimer approximation will be extremely accurate (the error is of the order of a fraction of a percent in the interaction energy), provided that there are no degenerate states (different states with the same energy) of the quasimolecule formed by the atoms a and b; this is the case of interest to us.

We note that the above expressions for χ, $Q^{(l)}$, and $\Omega^{(l,s)}$ involving $\varphi(R)$, as determined from the solution of the quantum-mechanical equation (6), are valid only for high enough temperatures, when the DeBroglie wavelength $\lambda_{DB} = 2\pi\hbar/(m_a v_a)$ of the interacting atoms is small compared to the size of the atoms and the distance between them. In this case classical mechanics can be used to treat the collision (we consider scattering by angles $\chi > \lambda_{DB}/b$) and then the formulas for χ, $Q^{(l)}$, $\Omega^{(l,s)}$, η, λ, and D_{12}.

At low temperatures, when λ_{DB}/b (or $\lambda_{DB}/\sigma \geqslant 1$), in the calculation of the transport coefficients and also the second virial coefficient, it is necessary to take into account quantum-mechanical corrections [1, 2, 11-14]. These corrections are determined by computing the $\Omega^{(l,s)}$ using the Schrödinger equation for the nuclear motion obtained in the Born–Oppenheimer approximation and using $\varphi(R)$ as the potential energy, as discussed above. Usually in these calculations, the $\varphi(R)$ used for the equation describing the nuclear motion is taken to be the empirical Lennard–Jones potential (4) [11-13], or the Kikhar potential [14]. The latter potential is called universal in [15] since it simultaneously describes the experimental data on viscosity, thermal conductivity, and other transport coefficients, as well as data on the second virial coefficient. For large λ_{DB}/σ it is necessary to take into account the symmetry properties dependent on whether the interacting atoms have integer spin (Bose–Einstein statistics) or half-integer spin (Fermi–Dirac statistics).

Quantum corrections of this kind are not very large (a few percent for low temperatures) and they are of practical interest only for helium and hydrogen at temperatures of order 10°K.

Below we consider the calculation of the transport coefficients based on the classical $\Omega^{(l,s)}$, but with the potential $\varphi(R)$ found quantum-mechanically. In the calculation of $\varphi(R)$ from (6) in the Born–Oppenheimer approximation, one usually applies the variational method of the self-consistent Hartree–Fock field with a linear combination of atomic orbitals and the Ruthaan equations [8-10]. The most accurate results are obtained with the inclusion of the configurational (or multiconfigurational) interaction, i.e., with the use of Slater determinants constructed from the single-electron wave functions of the ground state and several of the excited states of the system. In these calculations the Coulomb and exchange (corresponding to the Pauli exclusion principle* repulsion energies at small and intermediate

---

*Recall that according to this principle the electron wave function must be antisymmetric (must change sign upon permutation of any two electrons but keep the same absolute value). This requirement is satisfied when the Slater determinants are used.

interatomic distances are calculated, as well as the attractive energy, which reduces at large distances to the dispersion energy φ_{disp}. The dispersion attraction, also calculated independently in the second order of Rayleigh—Schrödinger perturbation theory, is due to the presence in the atoms (or molecules) of instantaneous dipoles and higher multipole moments arising from the motion of the electrons. The energy φ_{disp} for large distances can be represented in the form of a multipole expansion, in which each successive term is kept only if it is not larger than the prededing term [7, 10, etc]:

$$\varphi_{\text{disp}}(R) = -C_6R^{-6} - C_8R^{-8} - C_{10}R^{-10} - C_{12}R^{-12} - \dots \tag{8}$$

The energy φ_{disp} is calculated either by solution of the Schrödinger equation by variational methods with the inclusion of the configurational interaction, or with the help of perturbation theory (the former method is more accurate for intermediate distances). The dominant term in the multipole expansion (8) (valid at large distances) is the first (dipole—dipole) term. Methods of perturbation theory have also been developed for the calculation of the exchange interaction [10].

The determination of the interaction energy on the basis of the variational solution of the Schrödinger equation can be carried out without the use of any empirical parameters. This type of nonempirical calculation (ab initio — from the beginning) either with or without the configurational contribution can be done for the interactions of hydrogen atoms (in the formation of the diatomic molecule H_2), helium, and also alkali metal atoms between themselves and with inert gas atoms. We analyze the last case in this review.

In [16] the pairs Li—He and Na—He were considered* without taking into account configurational interaction, i.e., the electron interactions were taken to be the Coulomb and exchange interactions, which are most significant at small and intermediate internuclear distances. The first of these interactions leads to the mutual repulsion of the electrons and is taken into account in the expression for the energy by the corresponding Coulomb integral. In the core the integral includes the energy of attraction of the electrons to the nuclei. The repulsion of the nuclei does not affect the electron energies and can be taken into account separately. At intermediate and large distances its contribution to the interatomic energy is approximately cancelled by the averaged Coulomb repulsion of the electrons. At these distances the principal contribution is the exchange interaction, followed by the dispersion interaction. In calculations using the Hartree—Fock method, the exchange interaction due to the repulsion of electrons with parallel spins in correspondence with the Pauli principle is taken into account (this is equivalent to requiring that the wave functions be antisymmetric). In order to take into account the correlations of the electrons due to the repulsion of pairs of electrons with antiparallel spins, one must include the configurational interaction.

For the system metal atom—He atom, the contribution of the configurational interaction (which includes the dispersion attraction) is not large at intermediate distances since the polarizability of helium is small (an order of magnitude smaller, for example, than the polarizability of argon) and the coefficient C_6, which basically determines the dispersion energy, is proportional to the polarizability. For large internuclear distances the configurational interaction for the pairs H—He and Li—He is taken into account in [17]. Evidently the potential well depths are not very large. For example in the pair Li—He the depth of the potential well is about $0.07 \cdot 10^4$ a.e. =2.2°K for internuclear distance $R \approx 12$ a.e. = 6.35 Å (Fig. 1).† For large values of R the energy corresponds to the first two terms of the multipole expansion formula (8) (for Li—He C_6 = 23.8 a.e. and C_8 = 1261 a.e.) and for intermediate values of R the energy of attraction turns out to be less than according to (8) (in absolute value). In Fig. 1 we show (for $R < 10$ a.e.) the energy of repulsion according to [16] (without the configurational interaction). In this case the exchange repulsion is dominant (for values of $\varphi(R)$ around 10^{-3}-10^{-2} a.e., about 300-3000°K). Only for large R is the dispersion attraction the dominant contribution.

---

*In these calculations and the nonempirical and semiempirical calculations discussed earlier, the calculations are performed for the ground and excited states of the metal-inert-gas quasimolecule. In transport (diffusion) calculations, data for the ground state are used.

†For the pair H-He the depth of the potential well is (according to the calculation of [17] about $0.17 \cdot 10^4$ a.e. = 5.4°K for $R \approx 7$ a.e. = 3.7 Å.

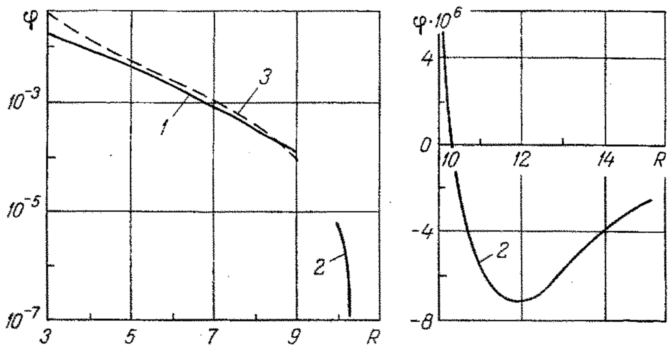

Fig. 1. Potential energy φ(a.e.) of the interaction of lithium and sodium atoms with helium atoms as a function of the internuclear distance R (a.e.) according to quantum-mechanical calculations: curve 1, lithium [16] (without the inclusion of the configurational interaction), curve 2, lithium [17] (with the inclusion of the configurational interaction) and curve 3, sodium [16] (without the configurational interaction).

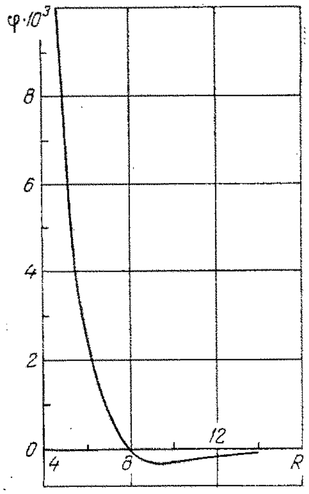

Fig. 2. Potential energy φ(a.e.) of the interaction of sodium atoms with argon atoms as a function of the internuclear distance R(a.e.) from the nonempirical quantum-mechanical calculations of [18] (with the inclusion of the configurational interaction).

Calculations of the complete interaction for small, intermediate, and large values of the internuclear distance with the inclusion of the Coulomb, exchange, and configuration interactions were carried out in [18] for the pair Na—Ar. In this case the contribution of the configurational interaction at small and intermediate distances is relatively large (see [19] for some illustrative graphs). The potential well in this case too turns out to be not very deep, about $0.24 \cdot 10^{-3}$ a.e. or 76°K at $R = 9$ a.e. (Fig. 2).

An approximate nonempirical calculation including the interaction of the electrons of the outer shells of the atoms (and the effect of the atomic cores with the use of appropriate pseudopotentials [20]) was carried out in [21] for the pairs Na—Ar and Na—Xe (with the inclusion of the configuration interaction). For Na—Ar, the value of φ(R) was about 1.3 times higher than in [18].

In addition to the nonempirical calculations, a series of semiempirical calculations have been published for alkali-atom-inert-gas-atom pairs. These calculations are done using the variational method with different simplified Hamiltonians. In [22] the Hamiltonian was represented as a sum of the Hamiltonian of the valence electron of the metal atom and the interaction potential energy of this electron and the core of the metal atom with the unperturbed inert gas atom. In the potential energy the electrostatic attraction of the electron to the inert gas atom (dipole) was taken into account (at large distances this interaction approaches the dispersion form with the potential proportional to R^{-6}) and also the repulsion between the electron and the inert gas atom and the repulsion between the core of the metal atom and the inert gas atom. In the calculation of the repulsive interaction, a pseudopotential of the Gombas [23] type is used, where the two terms of this pseudopotential correspond to the two types of repulsion discussed above. The pseudopotential is based on the Thomas–Fermi statistical model of the electron shells and is constructed such that the Pauli principle is satisfied, i.e., it antisymmetrizes the electron wave functions of the system. The repulsive interaction is an exchange interaction and dominates at small (or intermediate) internuclear distances, and while the electrostatic attraction dominates at large distances.

In the semiempirical calculations of [22] the free parameter r_0 was introduced (the equivalent radius of the inert gas dipole) which is much smaller than the internuclear distance R. It is chosen by matching the calculated potential well depth (for the ground state) with experiment, using the data of [24] from the scattering of an atomic beam of metal atoms into inert gases. In [25] this method was improved by increasing the number of states (ground state and excited states) of the alkali metal atom* included in the atomic base states. In [26, 27] improved results are given for the excited states of the metal–gas quasimolecule (in [26] graphs are given also for the ground state). The purpose of the calculations [22, 25-27] was to find the potential energy for the excited states using the experimental values of the potential well depths in the ground state.

Other semiempirical calculations for the pairs Li–He, Li–Ne, Na–He, Na–Ne are known; these calculations involve the use of an empirical potential in the Hamiltonian, obtained from experimental data on scattering of electrons by inert gas atoms and alkali metal ions [28-30]. Also considered is the interaction of the atomic core of the metal atom with an inert gas atom. The interaction of metal and gas atoms at large distances goes over into the dispersion interaction.

The nonempirical and semiempirical calculations of the interaction potential energy of alkali metal atoms with inert gas atoms were used in [19] to determine the diffusion coefficient of alkali metal vapors in inert gases. The interaction energy of the atoms (for the ground state of the quasimolecule) obtained in the various quantum-mechanical calculations, were approximated by the Monchik potential [3]

$$\varphi(R) = B\exp(-R/\delta), \tag{9}$$

where B and δ are constants. The use of the function (9), which does not have a potential well, is admissible because, for the cases considered in the calculation, the potential well depths are of the order of one degree (for mixtures with He; Fig. 1) or ten degrees (for mixtures with argon; for example; Fig. 2) and are small compared to the temperature for which the calculations are carried out. For (9) we have, according to [3]:

$$\sigma_{12}^2\Omega_{12}^{(1,1)*} = 4\alpha^2\rho^2 I(1,1), \tag{10}$$

where I(1, 1) is the collision integral for $l = 1$, $s = 1$ and is tabulated in [3] as a function $\alpha = \ln(B/kT)$. Further, in the calculations of D_{12} (or the quantities nD_{12} or PD_{12}, which are independent of the pressure) the formula (3) was used. If we replace the potential (9) with a power law dependence $\varphi(R) = B_1 \cdot R^{-n}$, where B_1 and n are constants [1], similar results are obtained. We emphasize that in any case the calculations for binary mixtures are carried out not on the basis of the combination rules, but directly from results applying to the interaction of unlike atoms.

---

*Recall that the inert gas atom is assumed to be unperturbed (since the interatomic collisions are thermal) and in the calculation of the dispersion energy this atom is treated as a dipole.

The calculated values of PD_{12} for mixtures of alkali metal vapors with inert gases are compared in [19] with the experimental data (or with calculations based on generalizations of the data; see below). The agreement is normally within the precision of the experimental data (usually ±10%) although in some cases the deviation is greater. If the starting point is made with sufficiently accurate quantum-mechanical calculations (for example [16] and in particular [18]) the agreement is better. Hence even purely theoretical calculations without the use of any experimental data give agreement with experiment.

The transport coefficients can also be calculated with the help of the asymptotic quantum-mechanical theory developed in [31-33]. We consider briefly the position of this theory as applied to the exchange interaction of an alkali metal atom with one relatively weakly bound (low ionization energy) valence electron and an inert gas atom. Then we apply this theory to calculate the interaction of an atom of a two-electron metal with an inert gas atom.

The Schrödinger equation for the wave function Φ of the valence electron of the unperturbed metal atom has the form

$$-\frac{1}{2}\nabla^2\Phi + V_M\Phi = E\Phi, \qquad (11)$$

where V_M is the interaction potential energy of the valence electron with the core of the metal atom (the part of the atom remaining after removal of the electron), and E is the energy of the metal atom. The wave function Ψ of this electron in the presence of a perturbation due to an inert gas atom satisfies a Schrödinger equation of the form

$$-\frac{1}{2}\nabla^2\Psi + V_M\Psi + V_G\Psi = E^s\Psi, \qquad (12)$$

where V_M is as defined previously and V_G is the interaction potential energy of the electron with the inert gas atom. The energy E^S of the ground state of the metal—gas quasimolecule is given by the expression

$$E^s = E + \varphi_{exch}(R), \qquad (13)$$

which does not include the energy of the inert gas atom, which is considered as a whole, since its electrons are bound to the nucleus because of the high ionization energies.

In order to find the exchange energy, equation (11) is multiplied by ψ and equation (12) by Φ and the two resulting equations are subtracted and integrated over a certain volume Ω including the inert gas atom (the functions Ψ and Φ are assumed to be real). In most of the region of interaction $V_G \approx 0$ and therefore $\Psi \approx \Phi$. Hence one can write

$$\int_\Omega V_\Gamma\Psi\Phi d\Omega = 0, \quad \int_\Omega \Psi\Phi d\Omega \approx \int_\Omega \Phi^2 d\Omega = 1,$$

since the functions Φ are orthonormal. Then with the help of Green's theorem the volume can be expressed in terms of an integral over a spherical surface surrounding the inert gas atom, and the exchange energy takes the form

$$\varphi_{exch} = \frac{1}{2}\Phi^2 \oint \nabla\Psi \cdot d\mathbf{S}, \qquad (14)$$

where dS is the intrinsic element of this surface. Here we have used the fact that near the surface the function Φ is slowly varying, and therefore $\nabla\Phi \approx 0$.

The wave function Ψ of the valence electron of the metal atom can be represented as a function centered at the nuclei of the metal and inert gas atoms [31]:

$$\Psi = \Phi(R) + \Phi_1(r_1) = \Phi(R) + C\exp(-\beta' r_1)/r_1, \qquad (15)$$

where r_1 is the distance from the inert gas nucleus to the valence electron of the metal atom, and $\beta' = \sqrt{\beta^2 - 2/R}$. The second term $\Phi_1(r_1)$ satisfies (approximately for $R \gg r_1$) the Schrödinger equation (11), in which the derivative in the Laplacian is taken with respect to the radius r_1. Also $V_M = -|R - r_1|^{-1} \approx -R^{-1}$, $E = -\beta^2/2 = -I_1$, where I_1 is the ionization potential of the metal atom. The quantity V_M determined in this way is the potential energy of the Coulomb attraction of the electron of the metal atom to its core. The interaction of the electron of the metal atom with the inert gas atom is taken into account by the constant C, which is determined below.

The wave function Φ(R) of the valence electron of an isolated metal atom also satisfies the Schrödinger equation (11) in which the derivative in the Laplacian is taken with respect to R. As before, $E = -\beta^2/2$, $V_M = -R^{-1}$. The asymptotic solution of this equation (for $\beta^2 R \gg 1$) has the form [31, 32]:

$$\Phi(R) = AR^{\frac{1}{\beta}-1} \exp(-\beta R)\, Y_{lm}(\theta, \vartheta), \tag{16}$$

where the $Y_{lm}(\theta, \vartheta)$ are the spherical functions, which characterize the angular (in spherical coordinates) distribution of the wave function of the electron with angular momentum l and component m of the angular momentum in some preferred direction. For s electrons (l = 0, m = 0), $Y_{00} = 1/\sqrt{4\pi}$; for p electrons (l = 1) $Y_{10} = \sqrt{3}/(\sqrt{4\pi}\cos\theta)$ for m = 0 but if θ = 0 then $Y_{10} = \sqrt{3}/\sqrt{4\pi}$. We can substitute $1/\sqrt{4\pi}$ for Y_{lm} and include the factor $\sqrt{2l+1}$ (which for l = 1 is equal to $\sqrt{3}$) separately.

The asymptotic coefficient A in (16) insures the matching of this solution with the Hartree–Fock solution for the valence electron of the atom. The value of A has been determined for metals and most other elements (usually to within ±10-20%) [31, 32, 34]. For the atoms indicated below, A takes the following values:

Li	Na	Zn	Cd	Hg	He	Ar
0,82	0,74	1,69	1,60	1,80	2,87	2,11

The constant C in (15) can be determined by using the scattering length L of the electron by the inert gas atom [31, 33, 35]. Then the electron wave function centered on the inert gas atom is written as:

$$\Psi' = N \exp(-r_1/L)/r_1, \tag{17}$$

where N is a constant. The average value of L (a.e.) from quantum-mechanical calculations and experimental data (on electron mobility in a gas, microwave scattering, etc.) are as follows for inert gas atoms:

He	Ne	Ar	Kr	Xe
1,2	0,2	—1,6	—3,2	—5,8

If for a known value of L we match the logarithmic derivatives of $r_1\Psi$ and $r_1\Psi'$ at a certain radius r_1 = ρ around the inert gas atom, i.e., we require the following boundary condition [31, 33]:

$$\frac{1}{r_1\Psi}\frac{d(r_1\Psi)}{dr_1}\bigg|_{r_1=\rho} = \frac{1}{r_1\Psi'}\frac{d(r_1\Psi')}{dr_1}\bigg|_{r_1=\rho} \equiv -\frac{1}{L}, \tag{18}$$

then we can find the value of the constant C.

Further calculations give Ψ and if we take ρ as the radius of integration in (14) then

$$\varphi_{exch} = 2\pi(L+\rho)(\beta'\rho+1)\,\Phi^2(R)/(1-\beta' L). \tag{19}$$

In order to refine the behavior of the wave function Ψ at distance ρ from the nucleus of the inert gas atom, the first term in (15) can be supplemented by the factor exp(β'ρ). More exactly (according to [31]) this factor (in the approximation $r_1/R \ll 1$) has the form $\exp(\beta' \cdot r_1 \cos\theta_1)$, where θ_1 is the angle between the direction r_1 and the axis R. We simply replace r_1 by ρ and take θ_1 = 0, since the exchange interaction at large R corresponds mainly to the region of electron coordinates near the internuclear axis [31]. Finally the factor exp(β'ρ) obtained in this way introduced directly into (19). In the calculations considered below [19] this factor is taken into account in φ_{exch} for ρ ≠ 0 and the results agree with those of the nonempirical calculations (only for values of ρ for the gas).

For helium, because of the small size of the helium atom, we take $\rho \approx 0$ in this case, then [31, 33]

$$\varphi_{\text{exch}} = 2\pi L \Phi^2(R)/(1 - \beta' L). \tag{20}$$

For $\beta' = 0$ we obtain the well-known Fermi formula. Equations (19) and (20) apply for $R > 2/\beta^2$, i.e., for realistic values of β'.

Equations (19) or (20), with (16) for $\Phi(R)$, can be used directly to determine the exchange interaction energy between atoms with a single valence electron (alkali metals) and helium atoms. It was shown in [19] that the value of $\varphi_{\text{exch}}(R)$ calculated in this way (for $\rho = 0$ and $L = 1.2$ a.e.) for the pairs Li–He and Na–He closely correspond (for $R > 2/\beta^2$) to the results of the nonempirical quantum-mechanical calculations of [16]. For metals with a large number of valence electrons it is necessary to include an additional factor ω in (19) or (20), which takes into account the difference of the quantum states of such an atom and its atomic core (with the electron removed) from the corresponding quantum states of a single-electron atom and its atomic core. This factor is calculated with the help of the genealogical scheme of Rak and has been applied to the case considered here in [31, 36]. The corresponding calculations for the interaction of two-electron atoms (of the type Zn, Cd, Hg) with a helium atom (or other inert gases) shows that $\omega = 2$. This value of ω is also valid for the interaction of two helium atoms. But for the interaction of two single-electron atoms or a single-electron atom and a two-electron atom (for example, an alkali metal atom and helium; see above) $\omega = 1$.

Calculation of the interaction energy of mercury atoms with inert gases (for $\omega = 2$) from the equation presented above, and with the inclusion of the dispersion energy φ_{disp} according to (8) and the general expression

$$\varphi(R) = \varphi_{\text{exch}}(R) + \varphi_{\text{disp}}(R)$$

leads to satisfactory agreement [19] with the values obtained from scattering data of atomic beams of mercury [37]. The same can be said about the correspondence of the calculated and experimental values of $\varphi(R)$ for the pairs Hg–Ne and Hg–Ar (for $\omega = 2$)*; $\rho = 1.1$ a.e. (for $L = 0.2$ a.e.) for the first pair and $\rho = 3.1$ a.e. (for $L = -1.6$ a.e.) for the second. If the latter values of ρ and L for argon) are used in the calculation of φ_{exch} of the pair Na–Ar from (19), then the results [19] for $R > 2/\beta^2$ correspond to those of [18] which were carried out without the inclusion of the configurational interaction.

The diffusion coefficients of zinc, cadmium, mercury, and sodium vapors in helium and argon, calculated with the asymptotic expression for $\varphi(R)$, closely correspond to the experimental data [19].

The asymptotic quantum mechanical theory has also been successfully applied to calculations of the interaction of alkali metal atoms and hydrogen [38]. The coefficients in the final formula, characterizing the interaction of the valence electron of the metal atom with the hydrogen atom, were fit (for the triplet and singlet states) to the results of the nonempirical quantum-mechanical calculations for lithium and hydrogen atoms [39]. These values also hold for the interaction of other alkali metals with hydrogen atoms. Then with certain approximations the cross sections $\sigma_{12}^2 \Omega_{12}^{(1,1)*}$ and $\sigma_{12}^2 \Omega_{12}^{(2,2)*}$ are found (with the inclusion of the dispersion attraction, where the values of the coefficients C_6 and C_8 are taken from the calculations of [40]) and these cross sections are used in the calculation of the transport coefficients in mixtures of monatomic alkali metal and vapors and atomic hydrogen.

The quantum-mechanical solutions considered above were nonrelativistic. Relativistic calculations of the electron shells of atoms with the use of the Dirac equation have been worked out [41–45]. In these papers all relativistic effects are taken into account, the principal one being the spin–orbit interaction, which is stronger the larger the charge Z of the nucleus of the atom (although the dependence is somewhat irregular). Because of relativistic effects, the electron shell of the atom is somewhat compressed (the average value of the electron coordinate r, its square r^2, and also the coordinate $r_{\max}$ of maximum electron density are all smaller in the relativistic treatment), while the maximum value of the wave functions

---

*With the inclusion of the additional factor $\exp(\beta'\rho)$ in equation (19) (for the mixtures Hg–Ne, Hg–Ar, and Na–Ar).

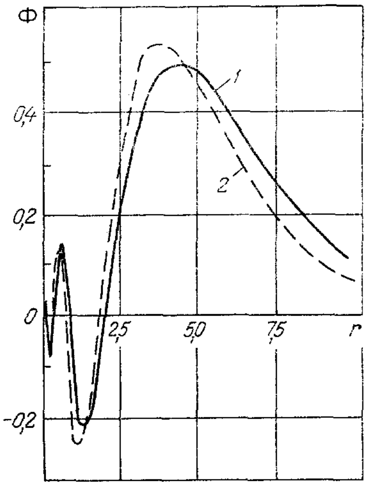

Fig. 3. Wave function Φ(a.e) of the valence 7s electron of uranium as a function of the distance r from the nucleus (a.e.) from nonrelativistic (curve 1) and relativistic (curve 2) calculations.

(orbitals) and hence the electron densities increase. For cesium (Z = 55), mercury (Z = 80), and uranium (Z = 92), the ratio a of the relativistic and nonrelativistic values of r_{max} for the outer orbital and the ratio b of the corresponding energies is [44]:

Atom	Orbital	*a*	*b*
Cs	6*s*	0,96186	1,03696
Hg	6*s*	0,85866	1,25661
U	7*s*	0,85685	1,21370

For $r > r_{max}$ the relativistic wave function (orbital) is smaller than the nonrelativistic. As an illustration we show in Fig. 3 the results for uranium [45]. Roughly the same picture must also hold for the 6s orbital of mercury (probably with a compression for smaller r approximately as the ratio of the quantities $\beta=\sqrt{2I}$, which for mercury and uranium is given by $0.876/0.670 \approx 1.3$). If we use (20) in the calculation of the potential energy of the exchange interaction of mercury atoms and helium, and take into account relativistic effects, then it is necessary to decrease the value of the asymptotic parameter A in (16). On average A must decrease by about 20% (for interatomic distances corresponding to interaction energies of mercury and helium atoms ranging from several hundred degrees to several thousand degrees).* This change in the parameter A (actually within the error of its determination in [31, 32, 34]) raises the calculated value of the diffusion coefficient of mercury vapor in helium by about 10% (for the same computational accuracy of D_{12}). For atoms with smaller values of Z the effect of the relativistic correlations to the diffusion coefficient are much smaller. In the semiempirical calculations [22, 25] of the interaction potential energy of alkali metal atoms with inert gas atoms, the relativistic spin–orbit interaction is taken into account approximately in the Schrödinger Hamiltonian in the usual way [7] (by introducing an additional small term).

It follows from the quantum-mechanical (nonrelativistic) relations discussed above that the interaction energies of atoms are determined mainly by the energies of the valence electrons (the quantities $\beta = \sqrt{2I}$) and the polarizabilities α of the atoms, since we have approximately $C_6=\frac{3}{2}\alpha_1\alpha_2\frac{I_1I_2}{I_1+I_2}$. This can be used to extend the values of the cross section $Q_{12}^{(l,l)}=\sigma_{12}^2\Omega_{12}^{(l,l)*}$ obtained from experimental data on diffusion of mixtures of metal vapors and gases, with the help of Eq. (3) [19, 46, 47]. For the reason indicated above, the ionization energies of the metal I_1 and gas I_2 are taken as units of measurement, as well as the polarizability of the gas α_2 (the value of α_1 is not required).

---

*In the determination of A in [31, 32, 34]; from the nonrelativistic wave functions the spectroscopic value of β was used for all elements.

An extensive series of experiments has been done on the determination of diffusion coefficients (by the Stefan method) for cesium, potassium, sodium, lead, zinc, mercury, cadmium, mangesium vapors in helium, argon, and molecular nitrogen [46-49]. Also the experimental data on the diffusion of chromium, manganese, iron, cobalt, and nickel in argon at high temperatures was used in [50]. The resulting generalized formulas can be used to calculate diffusion coefficients for mixtures not yet studied experimentally (to within an error not greater than the experimental error; usually about ±10%).

We discuss now the transport calculations in single-atom alkali metal vapors (without gas impurities) using the quantum-mechanical calculations of the atomic interactions. The results of the nonempirical quantum-mechanical calculations of the potential curves for two lithium atoms with the inclusion of the multiconfigurational interaction are given in [51, 52]. The viscosity and thermal conductivity of monatomic lithium vapor have been calculated in [53] using the calculations of [51, 52] with the inclusion of the triplet and singlet states. The potential curves was approximated by a repulsive exponential potential [3] (Eq. (9)) and an attractive potential of the same type [54].

The transport coefficients in monatomic alkali metal vapors have been calculated in [31, 55] using the asymptotic quantum-mechanical theory. In the quantum-mechanical calculations, a correction function is introduced into the unperturbed wave functions (16) of the valence electron. The correction function approaches unity when $R \to \infty$*. The calculations were simplified by assuming that the derivatives of the correction function with respect to the electron coordinates are much smaller than the derivatives of the unperturbed wave functions. Therefore these functions vary significantly at distances of the order of atomic dimensions, whereas the correction function varies notably only over distances of the order of the internuclear separation. For two widely separated identical atoms, each with one valence s-electron, the following expression is obtained in the asymptotic theory for the exchange splitting terms:

$$\Delta = BR^{\frac{7}{2\beta}-1} \exp(-2\beta R), \quad B = A^4 f(\beta), \tag{21}$$

where f(β) is the function of $\beta = \sqrt{2I}$, defined by a certain definite integral [31, 55].

With the inclusion of the dispersion attraction, the interatomic potential energy for large R is given as follows for the triplet and singlet states, respectively:

$$\varphi = \Delta/2 - C_6 A^{-6}, \quad \varphi = -\Delta/2 - C_6 R^{-6}. \tag{22}$$

Calculation of the collision integrals and transport coefficients [55] yields values which agree well with the corresponding experimental data; they either agree with the experimental values, or are somewhat higher than them (from 5% for cesium to 15-20% for sodium).

The disagreement between the calculated and experimental values of the transport coefficients of alkali metal vapors is usually explained by the effect of diatomic molecules (dimers) [5, 6, etc.]. The fraction of dimers in these vapors is not large, but the collision cross section between dimers and monomers is large, and this significantly affects the viscosity and thermal conductivity.† Values of the collision integrals (cross sections) have been given in [5, 6] with the effect of dimers taken into account.

The analysis of the experimental data on the transport coefficients for monatomic vapors is based on an extrapolation of the experimental values to zero pressure (where the dimer contribution must be zero). Analysis of the values given in the literature [5, 6, 56] can be used to determine the effective values of the parameters σ and ε of the Lennard-Jones potential (where these parameters take into account both the triplet and singlet interactions). If we again take the polarizability α and the ionization energy I as units, then it turns out that the ratios $\sigma/\alpha^{1/3}$ and ε/I are functions of the ionization energy (which is dimensionless in atomic units) [47]. For the inert gases [1], and also for mercury and zinc vapor [57], these dimensionless combinations are also functions of the ionization energy. Calculations of the viscosity and thermal conductivity of lithium vapor [47] with the use of the above dependences leads to practically the same results as the more complete theoretical calculations [53, 58].

---

*A similar method was used in [38] in the asymptotic calculation of the interaction of alkali metal atoms with hydrogen atoms.

†However the presence of dimers weakly affects the diffusion of monomers in mixtures with gases, particularly for low concentrations of metal vapor.

NOTATION

η, dynamic viscosity; λ, thermal conductivity; D_{12}, coefficient of mutual diffusion in a binary mixture; m, molecular mass of the single-component gas; k, the Boltzmann constant; T, absolute temperature; σ, geometrical parameter of the interaction potential energy φ of the molecules; ε, depth of the potential well; R, distance between atoms (or molecules) or the nuclei in the quantum-mechanical formulas; c_V, specific heat of the gas at constant volume; $n = P/kT$, total number of molecules per unit volume; P, total pressure; $m_{12} = m_1 m_2/(m_1 + m_2)$, reduced mass of two molecules of types 1 and 2; χ, angle of deflection (scattering) in the collision of molecules in the center of mass system; b, impact parameter; g, relative velocity of the molecules; R_m, distance of closest approach of the molecules during the collision; m_e and e, mass and charge of the electron; $\hbar = h/2\pi$, h = Planck's constant; m_a, mass of an atom; v_a, velocity of motion of an atom; φ_{exch} and φ_{disp}, exchange and dispersion interaction energies between atoms; I_1 and I_2, first ionization potentials (energies) for the metal and gas atoms; $\beta = \sqrt{2I_1}$; α_1 and α_2, polarizabilities of the metal and gas atoms; A, coefficient in the asymptotic electron wave function (16) (the asymptotic coefficient); L, scattering length of an electron by an atom; Δ, exchange splitting interaction energy of atoms with a single valence s-electron.

LITERATURE CITED

1. J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, Molecular Theory of Gases and Liquids, Wiley, New York (1954).
2. J. H. Ferziger and H. G. Kaper, Mathematical Theory of Transport Processes in Gases, Elsevier (1972).
3. L. Monchick, "Collision integrals for the exponential repulsive potential," Phys. Fluids, 2, No. 6, 695-700 (1959).
4. N. H. Davies, E. A. Mason, and R. T. Munn, "High-temperature transport properties of alkali metal vapors," Phys. Fluids, 8, No. 3, 444-452 (1965).
5. É. É. Shpil'rain, K. A. Yakimovich, É. E. Totskii, et al., Thermophysical Properties of Alkali Metals [in Russian], V. A. Kirillin (ed.) Standartov, Moscow (1970).
6. V. S. Yargin, N. I. Sidorov, and E. L. Studnikov, "Viscosity and thermal conductivity of alkali metals in a gas phase," Review of Thermophysical Properties of Materials, No. 5 (1978).
7. L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Pergamon Press, Oxford (1974).
8. G. M. Zhidomirov, A. A. Bagatur'yants, and I. A. Abronin, Applied Quantum Chemistry [in Russian], Khimiya, Moscow (1979).
9. V. I. Minkin, B. Ya. Simkin, and R. M. Minyaev, Theory of Molecular Structure (Electron Shells) [in Russian], Vysshaya Shkola, Moscow (1979).
10. I. G. Kaplan, Introduction to the Theory of Intermolecular Interactions [in Russian], Nauka, Moscow (1982).
11. L. Val'dman, "Transport phenomena in gases at moderate pressures," in: Thermodynamics of Gases [in Russian], Mashinostroenie, Moscow (1970), pp. 169-414.
12. A. G. Shashkov and T. N. Abramenko, Thermal Conductivity of Gas Mixtures [in Russian], Énergiya, Moscow (1970).
13. V. S. Yargin and L. I. Belashova, "Estimate of the quantum corrections to the transport coefficients of monatomic gases," Inzh.-Fiz. Zh., 27, No. 6, 1041-1045 (1974).
14. E. S. Barkan, "On the effect of quantum corrections to the second virial coefficient," Inzh.-Fiz. Zh., 42, No. 3, 495-496 (1982).
15. E. S. Barkan, "Universal intermolecular potential for nonpolar gases. 1. Inert gases," Zh. Tekh. Fiz., 54, No. 5, 1133-1150 (1984).
16. M. Krauss, P. Maldonado, and A. C. Wahl, "Interaction energy curves of LiHe and NaHe NaHe ($X^2\Sigma^+$, $A^2\Pi$, $B^2\Sigma^+$) and $X^1\Sigma^+$ Ions," J. Chem. Phys., 54, No. 11, 4944-4953 (1971).
17. G. Das and A. C. Wahl, "Theoretical study of the van der Waals forces in alkali-noble gas systems," Phys. Rev. A4, No. 3, 825-833 (1971).
18. R. P. Saxon, R. L. Olson, and B. Liu, "Ab initio calculations for the $X^2\Sigma$ and $B^2\Sigma$ states of NaAr," J. Chem. Phys., 67, No. 6, 2692-2702 (1977).
19. K. M. Aref'ev and M. A. Guseva, "Calculation of the diffusion coefficients of metal vapors in gases with the use of the quantum-mechanical solutions," Inzh.-Fiz. Zh., 47, No. 4, 608-617 (1984).
20. L. R. Kahn, P. Baybutt, and D. G. Truhlar, "Ab initio effective core potentials: reduction of all-electron molecular structure calculations involving only valence electrons," J. Chem. Phys., 65, 3826-3853 (1976).

21. B. C. Laskowski, R. S. Langhoff, and R. J. Stalicop, "Theoretical calculation of low-lying states of NaAr and NaHe," J. Chem. Phys., 75, No. 2, 815-827 (1981).
22. W. F. Baylis, "Semiempirical pseudopotential calculation of alkali-noble-gas interatomic potentials," J. Chem. Phys., 51, No. 6, 2665-2679 (1969).
23. P. Gombas, Pseudopotentiale, Springer-Verlag, New York (1967).
24. C. J. Malerich and R. J. Cross, "High energy alkali-rare-gas scattering," J. Chem. Phys., 52, No. 1, 386-393 (1970).
25. J. Pascale and J. Vandeplanque, "Excited molecular terms of the alkali rare gas atom pairs," J. Chem. Phys., 60, No. 6, 2278-2289 (1974).
26. E. Czuchaj and J. Sienkiewicz, "Adiabatic potentials of the alkali-rare gas atom pairs," Z. Naturforsch, A34, 694 (1979).
27. R. Düren and G. Moritz, "Improved model calculations for the alkali-rare gas," J. Chem. Phys., 73, No. 10, 5155-5159 (1980).
28. G. Bottcher, A. Dalgarno, and E. L. Wright, "Collision-induced absorption in alkali-metal-atom-inert-gas mixtures," Phys. Rev., 7, No. 5, 1606-1609 (1973).
29. J. Hansen, R. McCarrol, and P. Valiron, "Model potential calculation of the Na—He system," J. Phys. B, 12, No. 5, 899-908 (1979).
30. N. Phillips, F. Masnau-Seeuws, and P. Valiron, "Model potential method for the calculation of atom-rare-gas interactions. Application to the NaNe system," J. Phys., B, 12, No. 15, 2493-2510 (1979).
31. B. M. Smirnov, Asymptotic Methods in the Theory of Atomic Collisions [in Russian], Atomizdat, Moscow (1973).
32. V. M. Galitskii, E. E. Nititin, and B. M. Smirnov, Theory of Collisions of Atomic Particles [in Russian], Nauka, Moscow (1981).
33. M. Ya. Ovchinnikova, "Exchange bond of two unlike atoms at large distances," Zh. Eksp. Teor. Fiz., 49, No. 1 (7), 275-278 (1965).
34. A. A. Radtsig and B. M. Smirnov, Handbook of Atomic and Molecular Physics [in Russian], Atomizdat, Moscow (1980).
35. G. F. Drukarev, Collisions of Electrons with Atoms and Molecules [in Russian], Nauka, Moscow (1978).
36. E. L. Duman and B. M. Smirnov, "Exchange interactions of many-electron atoms," Opt. Spektrosk., 29, No. 3, 425-434 (1970).
37. T. R. Powers and R. J. Gross, "Molecular-beam determination of mercury rare-gas intermolecular potentials," J. Chem. Phys., 56, No. 6, 3181-3182 (1972).
38. É. É. Shpil'rain and A. Ya. Polishchuk, "Interaction potentials and collision integrals for hydrogen and alkali metal atoms," Inzh.-Fiz. Zh., 39, No. 6, 999-1004 (1980).
39. K. K. Docken and J. Hinze, "LiH potential curves and wavefunctions for $X^1\Sigma^+$, $A^1\Sigma^+$, $B^1\Pi$, ${}^2\Sigma^+$ and ${}^3\Pi^+$," J. Chem. Phys., 57, No. 11, 4928-4936 (1972).
40. T. R. Proctor and W. C. Stwalley, "The long-range interaction of s-state alkali atoms with rare gas and hydrogen atoms," J. Chem. Phys., 66, No. 5, 2063-2073 (1977).
41. I. P. Grant, "Relativistic self-consistent fields," Proc, R. Soc, 262A, 555-576 (1961).
42. M. A. Coulthard, "A relativistic Hartree—Fock atomic field calculation," Proc. R. Soc., 91, 44-49 (1967).
43. J. B. Mann and J. T. Waber, "Self-consistent relativistic Dirac—Hartree—Fock calculations of lanthanide atoms," At. Data, 5, 201-229 (1973).
44. J. P. Desclaux, "Relativistic Dirac—Fock expectation values for atoms with z = 1 to z = 120," At. Data Nucl. Data Tables, 12, 311-3046 (1973).
45. L. R. Kahn, P. J. Hay, and R. D. Cowan, "Relativistic effects in ab initio effective core potentials for molecular calculation of uranium," J. Chem. Phys., 68, 2386-2397 (1978).
46. K. M. Aref'ev, B. F. Remarchuk, and A. I. Galkin, "Diffusion of mercury vapor in gases," Inzh.-Fiz. Zh., 33, No. 3, 495-500 (1977).
47. K. M. Aref'ev, B. F. Remarchuk, and M. A. Guseva, "Extension of data on the diffusion of metal vapors in gases and transport properties of vapor," Inzh.-Fiz. Zh., 42, No. 6, 930-937 (1982).
48. K. M. Aref'ev, V. M. Borishanskii, L. A. Vorontsova, et al., "Diffusion coefficients of cesium, potassium, and sodium vapor in helium and argon," Teplofiz. Vys. Temp., 10, No. 5, 1112-1113 (1972).
49. K. M. Aref'ev, A. P. Lesyuis, B. M. Khomchenkov, and L. Sh. Tsemekham, "Features of diffuse condensation of zinc and lead vapor," Inzh.-Fiz. Zh., 27, No. 5, 825-832 (1974).
50. P. Grieveson and E. T. Turkdogan, "Determination of the interdiffusivities of argon and metal vapor mixtures at elevated temperatures," J. Phys. Chem., 68, No. 6, 1547-1552 (1964).

51. W. Kutzelnigg, V. Staemmler, and M. Gelus, "Potential curve of the lowest triplet state of Li_2," Chem. Phys. Lett., 13, No. 5, 496-500 (1972).
52. M. Olson and D. Konowalow, "Accurate potential energy curves for the $^3\Sigma_u^+$ and $^3\Sigma_g^+$ states of Li_2," Chem. Phys., 21, No. 3, pp. 393-399 (1977).
53. V. S. Yargin, N. A. Vanicheva, and V. I. Dolgov, "Transport coefficients of lithium in the gas state," Inzh.-Fiz. Zh., 39, No. 6, 993-998 (1980).
54. R. Brokaw, "Estimated collision integrals for the exponential attractive potential," Phys. Fluids, 4, No. 8, 944-946 (1961).
55. B. M. Smirnov and M. I. Chibisov, "Kinetic coefficients for monatomic alkai metal vapor," Teplofiz. Vys. Temp., 9, No. 3, 513-515 (1971).
56. N. B. Vargaftik, Handbook of Thermophysical Properties of Gases and Liquids [in Russian], 2nd ed., Nauka, Moscow (1972).
57. A. S. Umanskii, "Transport coefficients, second viral coefficients, and atom—atom interaction energies for Zn, Cd, and Hg vapors," Zh. Fiz. Khim., 46, No. 11, 2706-2709 (1972).
58. A. Ya. Polishuk, É. É. Shpil'rain, and I. T. Yakubov, "Thermal conductivity and viscosity of lithium," Inzh.-Fiz. Zh., 38, No. 3, 429-433 (1980).