Thermal conductivity prediction for nitrogen and carbon monoxide at the zero density regime via semi-empirically based assessment

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Thermal conductivity coefficients for gaseous states of N₂ and CO have been calculated by the inversion technique in conjunction with Wang Chang-Uhlenbeck-de Boer (WCUB) approach of the kinetic theory of gases for considering the various contributions of the molecular degrees of freedom to the thermal conductivity. The values of calculated thermal conductivity coefficients are commensurate with best experimental values.

Transport properties play an important role in many natural and technical processes. On the other hand, intermolecular forces are fundamental ingredients for both equilibrium and transport properties such as calculation of second virial coefficients, transport properties of simple fluids, integral equation theories, computer simulations, modified free volume theory (MFVT), and equation of state. Knowledge of pair interactions between molecules is of great importance in the theory of fluids. Hence, the application of the theory of fluids to real substances relies on the knowledge of the interactions between real molecules. Various methods of determining intermolecular potentials have been used, either theoretically, based on experimental information, or by combining both approaches. Among these methods, inversion of dilute gas properties has been of particular importance. For the noble gases, which have spherically symmetric interactions, inversion of transport properties data is directly related to the pair interaction potential \( u(r) \). For near-spherical and non-spherical molecules, inversion of transport properties gives an effective spherical potential \( u_{\text{eff}}(r) \) related to, but different from the true pair potential \( u(r, \omega) \) which depends on the intermolecular orientation, \( \omega \). Since these effective potentials are widely used in statistical mechanical calculations and chemical engineering applications, they have been determined approximately for many substances.

The experimental methods available for studying the properties of gases can be placed in one of the two broad categories, depending on whether they are concerned with measurements on a macroscopic or microscopic scale. In general, the calculated microscopic properties are more sensitive to the approximations used in a theory and to the assumptions made about the intermolecular potentials, but the macroscopic properties can be usually determined experimentally with greater accuracy. The two types of measurements are therefore complementary, each providing information that is useful in the development of a statistical-mechanical theory of gaseous state.

Working fluids and heat-transfer fluids circulating in refrigeration and heat-pump systems are often gases and hence there is a need for accurate values of the transport properties of gases. It is, therefore, necessary to replace direct measurement of transport properties by an alternative more accurate strategy designed to meet the same objective of a computer program. In order to substitute direct measurements, estimation schemes are being developed on the basis of the results of kinetic theory.

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 of extracting information about the intermolecular potential energy.
In the present work, the Wang Chang-Uhlenbeck-de Boer theory\textsuperscript{17} is applied to evaluate the various internal degrees of freedom to the thermal conductivity of CO and N\textsubscript{2} at zero density.

Theoretical

**Kinetic theory and pair-interaction intermolecular potential energy function**

The intermolecular interaction between two spherical molecules (or atoms) in the gas phase can be characterized in terms of a pair potential energy function \( U(r) \) which describes the overall result of (positive) repulsive energy between the molecules at small separations \( r \), the resultant (negative) attractive energy at larger distances, and the asymptotic approach of the resultant attractive energy to zero at very large separations. Two characteristic features of this function are\textsuperscript{7}, first, the separation at which the interaction energy passes through zero; this distance being referred to as the collision diameter \( \sigma \), and, second, the position of minimum interaction energy, \( U \), at which the interaction energy has a value \( -\epsilon \), where \( \epsilon \) is termed the well depth. If \( U(r) \) is known, the various transport properties of the system may be calculated by rigorous kinetic theory, which uses equations involving collision integrals, \( \Omega(l,s) \), which are integrals over the full range of energies, trajectories of collision, and orientations of molecules during collisions. It should also be mentioned that the indices, \( l,s \), specify weighting factors related to the mechanism of transport by molecular collisions. Chapman-Enskog solution of the Boltzmann kinetic equation for dilute monatomic gases relates these coefficients to a series of collision integrals \[ \text{ref. 19} \]. The collision integrals, \( \Omega(l,s) \), are defined as\textsuperscript{18}:

\[
\Omega(l,s)^{(l,s)} = \int_0^{\infty} Q(l) (E) e^{-E/kT} dE \quad \ldots(1)
\]

where \( E \) is the relative energy of colliding partners. The \( Q(l) \) is a transport collision integral that is classically given by Eq. (2).

\[
Q(l) = \left\{ 1 + \frac{(-1)^l}{2(l+1)} \right\} \int_0^{\infty} (1 - \cos \theta) b db \quad \ldots(2)
\]

where \( \theta \) is the relative scattering angle between two colliding partners of energy \( E \) and impact parameter \( b \) at the gas temperature.

The scattering angle, \( \theta \), is calculated as a function of \( b \) and \( E \) from Eq. (3).

\[
\theta(b,E) = \pi - 2b \left[ \frac{1}{r^2} - \frac{r}{U(r)}/E \right]^{1/2} dr/r^2 \quad \ldots(3)
\]

where the distance of closest approach, \( r_o \), is the outermost root of

\[
1 - b^2/r_o^2 - U(r_o)/E = 0 \quad \ldots(4)
\]

It is worth noting that the three successive numerical integration (i.e., Eqs 1-3) are required to obtain the collision integral. Numerical differentiation and use of the recursion relation can generate collision integrals higher than that mentioned\textsuperscript{18}.

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

where the reduced collision integral is defined by\textsuperscript{18},

\[
\Omega^{(l,s)*} = \Omega^{(l,s)}/\pi \sigma^2 \quad \ldots(6)
\]

where \( \sigma \) is the length scaling factor such that \( U(\sigma) = 0 \). The reduced temperature (\( T^* \)) is\textsuperscript{18}

\[
T^* = kT/\varepsilon \quad \ldots(7)
\]

and \( \varepsilon \) is the energy scaling factor.

The kinetic theory expression for the thermal conductivity coefficient of a pure monatomic dilute gas of molecular mass, \( m \), at the temperature, \( T \), is\textsuperscript{18}

\[
\lambda(T) = \frac{75}{64\pi^2} \frac{(k_B T / \pi m)^{1/2}}{\Omega^{(2,2)*}} \quad \ldots(8)
\]

Here \( k_B \) is the Boltzmann constant and \( \Omega^{(2,2)*} \) the reduced thermal conductivity collision integral.

**Thermal conductivity**

Transport coefficients describe the process of relaxation to equilibrium from a state perturbed by application of temperature, pressure, density, velocity or composition gradients. The kinetic theory of gases
yields theoretical expressions for the viscosity, thermal conductivity and other transport coefficients for gases, the results of which are in reasonably good agreement with experiment.

According to the Wang Change-Uhlenbeck-de Boer (WCUB) version of the kinetic theory of gases, each molecular degree of freedom contributes separately to the thermal conductivity and hence the thermal conductivity is written as a sum of contributions from translational, rotational, vibrational and electronic degrees of freedom.

\[ \lambda^{(0)} = \lambda^{(0)}_{tr} + \lambda^{(0)}_{rot} + \lambda^{(0)}_{vib} + \lambda^{(0)}_{ele} \]  \hspace{1cm} (9)

To a first approximation these contributions are independent except for translational and rotational contributions whose interaction must be taken into account. Moreover, the translational contribution is like that of a monatomic gas and the other contributions correspond to the transport of molecular internal energy by a diffusion mechanism, i.e., each internal degree of freedom is approximated by the mass diffusion coefficient, \( D \). It should be mentioned that electronic energy rarely plays any role and it is therefore a reasonable approximation to take the electronic degrees of freedom as independent and to take \( D_{ele} \approx D \). Also, it is a good approximation to take \( D_{vib} \approx D \).

So, the problem of prediction of thermal conductivity using WCUB theory is reduced to the determination of the translational-rotation interactions and the diffusion coefficients for rotational energy. Translation-rotation interaction is denoted by \( \zeta_{rot} \), called rotational relaxation. Mason and Uribe calculated the behavior of \( D_{rot} \) from \( \zeta_{rot} \).

The needed formulas for the calculation of \( \lambda \) are given below:

\[ \frac{m \lambda^{(0)}_{vib}}{\eta^{(0)}_{rot} k_B} = \frac{6}{5} A \frac{C_{vib}}{k_B} \]  \hspace{1cm} (10)

\[ \frac{m \lambda^{(0)}_{ele}}{\eta^{(0)}_{rot} k_B} = \frac{6}{5} A \frac{C_{ele}}{k_B} \]  \hspace{1cm} (11)

\[ \frac{m \lambda^{(0)}_{rot}}{\eta^{(0)}_{rot} k_B} = \frac{5}{2} \left( \frac{3}{2} - \Delta_{rot} \right) (1 + \Delta_{spin}) \]  \hspace{1cm} (12)

\[ \frac{m \lambda^{(0)}_{ele}}{\eta^{(0)}_{rot} k_B} = \frac{\rho D_{rot}^{ex}}{\eta^{(0)}_{rot}} \left( \frac{C_{rot}}{k_B} + \Delta_{rot} \right) (1 + \Delta_{spin}) \]  \hspace{1cm} (13)

\[ \frac{A'}{\rho^{(2,2)}_{rot}} = \Omega^{(2,2)}_{rot} \left( \frac{\rho D_{rot}^{ex}}{\eta^{(0)}_{rot}} \right)^{4/3} \]  \hspace{1cm} (14)

\( D_{rot}^{ex} \) is the diffusion coefficient for rotational energy with a correction for resonant exchange included. The correction terms \( \Delta_{rot} \) and \( \Delta_{spin} \) are

\[ \Delta_{rot} = \frac{2}{\pi \zeta_{rot}} \frac{C_{rot}}{k_B} \left( \frac{5}{2} \frac{\rho D_{rot}^{ex}}{\eta^{(0)}_{rot}} \right) \]  \hspace{1cm} (15)

\[ \Delta_{spin} = \left( 1 + \frac{8}{15 \pi \zeta_{rot}} \frac{C_{rot}}{k_B} \rho D_{rot}^{ex} \right) \left( \frac{3 C_{rot}}{5 k_B} \right) \]  \hspace{1cm} (16)

\( C_{vib} \) was estimated by Eq. 17 obtained from statistical mechanics:

\[ C_{vib} = \frac{\sum_{j=1}^{k} (\Theta_{vj} / T)^2 \exp(-\Theta_{vj} / T)}{1 - \exp(-\Theta_{vj} / T)} \]  \hspace{1cm} (17)

Here, the symbol \( \Theta_{vj} \) identifies the characteristic vibrational temperature for the vibrational degree of freedom, \( j \) [ref. 21].

The temperature dependence of \( \zeta_{rot} \) is given by:

\[ \zeta_{rot}^{ex} = 1 + \frac{\pi^{3/2}}{2 (T^*)^{1/2}} \left( 2 + \frac{\pi^2}{4} T^* \right) \frac{1}{(T^*)^{3/2}} \]  \hspace{1cm} (18)

The correlation for \( D_{rot} \) in terms of \( \zeta_{rot} \) is given in two parts: a low-temperature part [ref. 20], which switches to high temperature results at a reduced crossover temperature \( T^* \) [ref. 20].

For \( T^* \leq T^{cross} \)

\[ \frac{\rho D_{rot}^{ex}}{\eta^{(0)}_{rot}} = \left( \frac{\zeta_{rot}}{\zeta_{rot}^{ex}} \right)^{3/4} \left( 1.122 + 4.552 / T^* \right) \]  \hspace{1cm} (19)

For \( T^* \geq T^{cross} \)
The resonant energy exchange corrections to $D_{rot}$ depend on the molecular dipole and quadrupole moments.

\[
\frac{\rho D_{rot}}{\eta^{(0)}} = \frac{\rho D^{(0)}}{\eta^{(0)}} \left( 1 + 0.27/\zeta_{rot} - 0.44/\zeta_{rot}^2 - 0.90/\zeta_{rot}^3 \right)
\]

\ldots (20)

where $\zeta_{rot}$ is the characteristic rotational temperature, in which $I$ is the molecular moment of inertia. The quantities $g^{\mu \rho}$, $g^{\mu \mu}$, $g^{\rho \rho}$ are dimensionless factors of order unity that correct for the replacement of quantum-mechanical summations by integrations. Their high-temperature asymptotic forms are:

\[
g^{\rho \rho} = \exp \left( -13\theta_{rot} / 6T \right) \left[ 1 - (4\theta_{rot} / 3T) + \ldots \right] \ldots (25)
\]

\[
g^{\mu \mu} = \exp \left( -17\theta_{rot} / 12T \right) \left[ 1 - (5\theta_{rot} / 6T) + \ldots \right] \ldots (26)
\]

\[
g^{\mu \rho} = \exp \left( -2\theta_{rot} / 6T \right) \left[ 1 - (\theta_{rot} / 3T) + \ldots \right] \ldots (27)
\]

which are sufficiently accurate for most purposes. It should also be noted that in the aforesaid equations, $\eta^{(0)}$ and $D^{(0)}$ are the viscosity and self-diffusion coefficients at zero density.

**Inversion technique**

The inversion method has been depicted in detail in Fig. 1.

In the present study, the three consecutive integrals, i.e., Eqs (1-3), are evaluated using the numerical integration and computer program developed by O'Hara and Smith\textsuperscript{22}. It may also be pointed out that the integral of deflection angle, i.e., Eq. (3), is integrated by trapezium rule. The cross-section, i.e., Eq. (2), and the collision integrals, i.e., Eq. (1), are evaluated by using a Gauss-Legendre quadrature (i.e. numerical integration)\textsuperscript{50-53}. The literature and calculated values of the thermal conductivity are given in Figs 2 and 3. In the present work, the collision integrals and their ratios for CO and N\textsubscript{2} systems are given in Table 1.

**Results and Discussion**

As mentioned earlier, the problem of obtaining the interaction potential energy is the calculation of force by analyzing the bulk properties. The degree of success will depend on the accuracy and sensitivity of the measurements as well as the theory connecting the force to macroscopic properties. The transport coefficients of dilute gases, especially viscosity, which depends on binary interaction, satisfy the above condition. It is worth noting that the terms dilute or low-density gas represent a real physical situation, whereas the frequently-used expression zero-density limit is related to results of a mathematical extrapolation of a density series of a particular transport property at constant temperature to zero density. The derived value is assumed to be identical with the true value for the dilute-gas state, which in most cases turns out to be correct. In this respect, the inversion procedure plays an important role for generating a like-molecule potential from the viscosity data and their corresponding states correlation. In the case of the corresponding states principle, it must be mentioned that since the functional equation obtained from this principle applies in a more limited form to molecular gases than to noble gases, the arithmetic mean of the functions should be used for the components of gas mixtures. Also, we are confined only to $T^* \geq 1.0$, because viscosity collision integrals for molecular gases at low temperatures do not exist. Consequently, in order to proceed to the next iteration it is necessary to extrapolate $U(r)$ in the long-range region (low temperature). The extrapolation function that we have used is $V^* = -C_6 u^6$, where $C_6$ is the dispersion coefficient and $u$ is the reciprocal of the intermolecular distances, both in atomic units. It is to be noted that the inversion procedure is not unduly
sensitive to the nature of the extrapolating function. 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 $V = -C_6 u^6$ as extrapolating function at long range region, the inversion function procedure is not unduly sensitive to the nature of the extrapolating functions used. This is due to the fact that the potential will adjust itself during iteration steps (as depicted in the flow chart). As mentioned before, the inversion function $G_\eta(T)$ is found to be remarkably

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**Fig. 1** — Schematic diagram for the INVERSION procedure.

**Fig. 2** — Deviation values of thermal conductivity for CO. [The experimental values are taken from ref. 25].

**Fig. 3** — Deviation values of thermal conductivity for N$_2$. [The experimental values are taken from ref. 25].
insensitive to the precise nature of the potential, a
text which greatly enhances the convergence rate
of the inversion. It is worthwhile to note that for a
given transport property, $G_\eta(T^*)$ is determined by the

\[
\begin{align*}
A^* &= \frac{\Omega^{(2,1)*}}{\Omega^{(1,1)*}}, \\
B^* &= \frac{5\Omega^{(1,2)*} - 4\Omega^{(1,3)*}}{\Omega^{(1,1)*}}, \\
C^* &= \frac{\Omega^{(1,2)*}}{\Omega^{(2,3)*}}, \\
E^* &= \frac{\Omega^{(3,3)*}}{\Omega^{(1,1)*}}, \\
F^* &= \frac{\Omega^{(2,2)*}}{\Omega^{(1,1)*}} 
\end{align*}
\]

Table 1 — The reduced collision integrals and their ratios for the N$_2$ and CO systems.

<table>
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<tr>
<th>Log $T^*$</th>
<th>$&lt;\Omega^{(1,1)*}$</th>
<th>$&lt;\Omega^{(2,2)*}$</th>
<th>$A^*$</th>
<th>$B^*$</th>
<th>$C^*$</th>
<th>$E^*$</th>
<th>$F^*$</th>
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| CO system |
| 0.0 | 1.4104 | 1.5724 | 1.1149 | 1.2018 | 0.8453 | 0.8771 | 0.9201 |
| 0.1 | 1.2718 | 1.4085 | 1.1076 | 1.1698 | 0.8561 | 0.8849 | 0.9266 |
| 0.2 | 1.1569 | 1.2737 | 1.1010 | 1.1434 | 0.8703 | 0.8972 | 0.9360 |
| 0.3 | 1.0633 | 1.1661 | 1.0967 | 1.1240 | 0.8856 | 0.9113 | 0.9471 |
| 0.4 | 0.9875 | 1.0815 | 1.0952 | 1.1114 | 0.9000 | 0.9249 | 0.9587 |
| 0.5 | 0.9256 | 1.0150 | 1.0966 | 1.1047 | 0.9123 | 0.9369 | 0.9696 |
| 0.6 | 0.8742 | 0.9620 | 1.0905 | 1.1028 | 0.9218 | 0.9463 | 0.9792 |
| 0.7 | 0.8303 | 0.9187 | 1.0855 | 1.1046 | 0.9286 | 0.9533 | 0.9874 |
| 0.8 | 0.7915 | 0.8821 | 1.1145 | 1.1097 | 0.9325 | 0.9581 | 0.9939 |
| 0.9 | 0.7559 | 0.8500 | 1.1244 | 1.1181 | 0.9340 | 0.9611 | 0.9989 |
| 1.0 | 0.7220 | 0.8206 | 1.1364 | 1.1295 | 0.9330 | 0.9621 | 1.0031 |
| 1.1 | 0.6888 | 0.7920 | 1.1499 | 1.1412 | 0.9301 | 0.9603 | 1.0076 |
| 1.2 | 0.6554 | 0.7619 | 1.1625 | 1.1483 | 0.9261 | 0.9548 | 1.0136 |
| 1.3 | 0.6220 | 0.7280 | 1.1704 | 1.1456 | 0.9230 | 0.9462 | 1.0209 |
| 1.4 | 0.5896 | 0.6989 | 1.1700 | 1.1308 | 0.9225 | 0.9369 | 1.0278 |
| 1.5 | 0.5594 | 0.6486 | 1.1595 | 1.1065 | 0.9261 | 0.9302 | 1.0324 |
| 1.6 | 0.5328 | 0.6075 | 1.1402 | 1.0775 | 0.9339 | 0.9287 | 1.0336 |
| 1.7 | 0.5109 | 0.5698 | 1.1153 | 1.0495 | 0.9448 | 0.9330 | 1.0315 |
| 1.8 | 0.4938 | 0.5378 | 1.0889 | 1.0260 | 0.9571 | 0.9421 | 1.0275 |
ratio of the impact parameter to the distance of closest approach for a collision at an energy $\geq (s + 1)kT$ which results in a deflection angle of $\theta \sim \pi/2$. Herein, $s$ has its usual meaning which has been pointed out in previous section (§ Kinetic theory and pair-interaction intermolecular potential energy function). In order to maintain this deflection angle constant as the potential changes, the impact parameter needs to be changed; the distance of closest approach will change in the same direction and by roughly the same magnitude for this small deflection angle, while the impact parameter and the distance of closest approach are similar. One therefore expects their ratios, and hence the $G_\eta(T^*)$ function (and consequently extrapolating function), to be essentially independent of the precise nature of the potential.

The vibrational frequencies necessary for calculating the vibrational part of the thermal conductivity were taken from McQuarrie. It may be noted that the contribution to $\lambda_{\text{elec}}$ is small because the corresponding contributions to the heat capacity are small for the range of temperatures considered here. Therefore, in the present study, we neglected the term $\lambda_{\text{elec}}$.

The terms $\Delta_{\text{ex}}$ and $\Delta_{\text{ex}}^\text{rot}$ are zero for nitrogen molecule because it does not have (permanent) dipole moment. Therefore, for a given temperature, the first step is the calculation of $\zeta_{\text{rot}}$ and $D_{\text{rot}}$ from Eqs. 18 and 19 or 20. $D_{\text{rot}}$ can be used to calculate $D_{\text{rot}}^\text{ex}$ from Eqs. 21–27. From $\zeta_{\text{rot}}$ and $D_{\text{rot}}$, $\Lambda_{\text{rot}}$ and $\Delta_{\text{spin}}$ are calculated using Eqs (15) and (16). Applying $D_{\text{rot}}^\text{ex}$ and $\Delta_{\text{rot}}$ values to Eqs. (10)-(13), the thermal conductivity $\lambda$ can be computed. It should also be noted that the viscosity coefficient $\eta^{(0)}$ and self-diffusion coefficient $D^{(0)}$ at zero density needed in the calculation of the thermal conductivity coefficient were taken from the present calculations.

### Conclusions

The present study describes an interesting application of the inversion method. The accuracies of the calculated transport properties arise from the intermolecular potential energy obtained from the inversion procedure. In the present study, the direct inversion procedure has been applied to corresponding states of viscosity given by Bzowski et al. to generate a unique spherically effective pair potential energies which are reliable. This is based on the fact that the revision of the extended principle of the corresponding states by Bzowski et al. correlates the viscosity of the molecules and their mixtures at low density over a very wide temperature range with very good accuracy. It also characterizes each binary interaction with the aid of five classical-material parameters $\sigma$, $\varepsilon$, $\rho^*$, $C_6^*$, and $U_0^*$. With the effective potential energy function, improved collision integrals have been obtained which are needed for the calculation of the transport properties. The main advantage of the ratios of the collision integrals obtained from the inversion of the corresponding states of viscosity is that it is more accurate than those obtained from other corresponding states because measurements of viscosity is more practical than those of other transport properties.

Thermal conductivity calculated from the INVERTED potential by the of WCUB approach, and subsequent comparison with the experimentally based values, has been shown to provide a powerful test of accuracy of INVERTED potential. This scheme provides accurate potential energy and allows determination of collision integrals more accurately than is possible by the extended law of corresponding states. The direct inversion of the viscosity collision integral correlation obtained from an extended law of corresponding states is obviously a powerful method for establishing an accurate unlike-pair potential energy. The accurate potential energy obtained by inversion of viscosity data can reproduce (within precision of the experimental data) all transport properties. Based on the present study, we propose that the inclusion of the WCUB approach of the kinetic theory of gases for considering the various contributions of the molecular degrees of freedom to the thermal conductivity is reasonable. The deviation obtained here is of the same order as those obtained by other authors. The estimated accuracy is also commensurate with the best measurements of thermal conductivity, i.e., 12%.
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Symbols used

- $b$: impact parameter
- $l$, $s$: specify weighting factors related to the mechanism of transport by molecular collisions
- $r$: intermolecular distance
- $k$: Boltzmann constant
- $m$: molecular mass
- $u$: reciprocal of the intermolecular distance
- $C_6$: dispersion coefficient
- $G$: inversion function
- $T$: absolute temperature
- $V(r)$: intermolecular potential energy
- $A^*, B^*, C^*, E^*, F^*$: ratios of collision integral
- $T^*$: reduced temperature
- $Q^0(E)$: transport collision integral
- $D^{(0)}$: self-diffusion coefficient at zero density
- $D_{rot}$: coefficient for diffusion of molecular rotational energy
- $D_{vib}$: coefficient for diffusion of molecular vibrational energy
- $D_{elec}$: coefficient for diffusion of molecular electronic energy
- $D_{rot}^{*}$: diffusion coefficient for rotational energy including correction for resonant exchange
- $C_{vib}$: molar heat capacity due to molecular vibration
- $C_{rot}$: molar heat capacity due to molecular rotation
- $C_{elec}$: molar heat capacity due to molecular electronic degrees of freedom
- $G^{μμ}$: temperature-dependent dimensionless factor needed in calculation of $Λ_{rot}^{μμ}$
- $G^{μ0}$: temperature-dependent dimensionless factor needed in calculation of $Λ_{vib}^{μ0}$
- $G^{00}$: temperature-dependent dimensionless factor needed in calculation of $Λ_{elec}^{00}$
- $v$: energy scaling factor
- $σ$: length scaling factor
- $θ$: relative scattering angle between two colliding partners
- $Ω^{(l,s)}$: collision integral
- $Ω_{rot}^{(l,s)}$: reduced collision integral
- $Ω_{vib}^{(1,1)}$: reduced collision integral for diffusion
- $Ω_{elec}^{(2,2)}$: reduced collision integral for viscosity (or thermal conductivity)
- $η^{(0)}$: viscosity coefficient at zero density
- $Z^{(0)}$: thermal conductivity at zero density
- $λ_{vib}^{(0)}$: contribution of molecular translational energy to thermal conductivity at zero density
- $λ_{rot}^{(0)}$: contribution of molecular rotational energy to thermal conductivity at zero density
- $Λ_{vib}^{μ0}$: contribution of molecular vibrational energy to thermal conductivity at zero density
- $Λ_{elec}^{00}$: contribution of molecular electronic energy to thermal conductivity at zero density
- $Δ_{rot}^{μμ}$: correction for resonant exchange of molecular rotational energy due to dipole-quadrupole interactions
- $Δ_{vib}^{μ0}$: correction for resonant exchange of molecular rotational energy due to quadrupole-quadrupole interactions
- $Δ_{elec}^{00}$: correction for resonant exchange of molecular rotational energy due to dipole-dipole interactions
- $z_{rot}$: collision number for rotational relaxation
- $z_{vib}^{∞}$: high-temperature asymptotic value of collision number for rotational relaxation
- $Δ_{rot}$: correction to $λ$ for interaction of molecular rotational and translational energy
- $Δ_{vib}$: correction to $λ$ for alignment of molecular angular momentum (spin polarization)
- $Θ$: quadrupole moment
- $θ_{vib} = \hbar^2/2kl$: characteristic rotational temperature
- $θ_{rot}$: characteristic vibrational temperature
- $ρ$: mass density of gas

References


