

Transport Properties of Non-Spherical Gases

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Transport properties of dilute gases consisting of non-spherical molecules are described in this work via permanent and induced electric multipole moments. We separated the part dependent on the angular variables and considered it as a perturbation to the central-type intermolecular potential energy. The spherically symmetric component of the potential function was assumed to be the Lennard–Jones 12–6 form. In this work, we obtained the general expressions for non-central contributions to the collision integrals. These expressions were applied to cases of axially symmetric with respect to the z -axis. Numerical examples of the effects of non-spherical interactions are given for NO and CO.

Accurate knowledge of transport properties of fluids is important for determining intermolecular potential energy functions, and for the optimal design of the chemical process plants. These properties for dilute monoatomic gases were calculated from the Enskog–Chapman kinetic theory. The kinetic theory of polyatomic molecules, which take into account of inelastic collision, are extremely complex, and there have been only a few attempts to calculate the transport properties from this theory.^{1–5} The Chapman–Enskog theory gives, however, a satisfactory description for the case of viscosity and diffusion coefficients only if the gas consists of atoms or molecules that can be treated as sphere interacting centrally.^{6–11} While much progress has been made in describing the thermodynamic properties of assemblies of molecules with spherical symmetry, there are many molecules, of which the force fields depend on relative orientations. The problem becomes highly involved if the gas consists of molecules having a complex electronic structure. In other word, it is no longer possible to use a spherical approximation, since their interaction potential depends not only on their distances, but also on their mutual orientations. The Mason–Monchick approximation, however, has been developed to calculate the transport coefficients of polyatomic molecules.^{12–14} This approximation is based on the assumption that the Chapman–Enskog theory of polyatomic molecules retains its original form, but the collision integrals must be averaged over all possible relative orientations occurring in the collisions. Their classical model ignores inelastic collisions, restricting its applicability to viscosity and diffusion coefficients and also to translational part of thermal conductivity, and then, the collision integrals can be calculated assuming that molecules collide with a fixed relative orientation during the encounter. Tests of the Mason–Monchick approximation carried out on the atom–molecule systems have shown to agree within 3%,^{15,16} but it can be shown that for linear molecule–molecule systems the deviations are up to 10%.¹⁷

In this work, we separated the part dependent on the angular variables and considered it as a perturbation to the central-type intermolecular potential energy. Thus, investigation of the collision integrals made it possible to determine not only the pa-

rameters of the central forces but also yielded information concerning the electric multipole moments of the molecules, since angular dependence of the potential energy arises primarily from electric multipoles in the molecule. The theoretically derived non-central contributions to collision integrals were valid in general for molecules of arbitrary symmetry and arbitrary electrical structure; the obtained expressions were applied to two cases of axially symmetric, CO and NO.

Theory and Calculation

In the limit of zero density, the transport coefficients of a gas can be expressed, using kinetic theory, in terms of collision integrals $\Omega^{(l,s)}(T)$, which are related to the intermolecular potential energy $u(r, \omega_a, \omega_b)$ between two molecules a and b that are separated by distance r and having the orientations specified by ω_a and ω_b .¹⁸

$$\chi(b^*, E^*) = \pi - 2b^* \int_0^\infty \frac{r^{*2} dr^*}{\{1 - (b^{*2}/r^{*2}) - [u^*(r^*, \omega_a, \omega_b)/E^*]\}^{1/2}}, \quad (1)$$

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

$$\Omega^{(l,s)*}(T^*) = \frac{[(s+1)! T^{*(s+2)}]^{-1}}{\int_0^\infty Q^{(l)*}(E^*) \exp\left(\frac{-E^*}{T^*}\right) E^{*(s+1)} dE^*}, \quad (3)$$

where for viscosity and thermal conductivity, $l = 2$ and $s = 2$, and for diffusion, $l = 1$ and $s = 1$. In these expressions, χ is the scattering angle, $Q^{(l)*}(E^*)$ is the reduced transport collision integral as a function of reduced kinetic energy $E^* \equiv E/k_B T$, and the reduced impact parameter $b^* \equiv b/\sigma$, $r_0^* \equiv r_0/\sigma$ is the closest approach of two molecules, where σ is a distance scaling parameter, $u^* \equiv u/\varepsilon$ and $T^* \equiv k_B T/\varepsilon$, in which ε is potential well and k_B is Boltzmann constant. Thus, three successive integrations can be performed once the intermolecular pair potential energy is known. The kinetic theory expressions for viscosity (η_{12}) and the binary diffusion coefficient (D_{12}) in terms of

collision integrals $\Omega^{(l,s)}(T)$ are as follow:

$$[\eta_{12}]_1 = \frac{5}{16} \left(\frac{2m_1 m_2 k_B T}{(m_1 + m_2) \pi} \right)^{1/2} \frac{1}{\sigma_{12}^2 \Omega_{12}^{(2,2)*}(T_{12}^*)} f_\eta, \quad (4)$$

$$D_{12} = \frac{3}{8} \left[\left(\frac{m_1 + m_2}{2m_1 m_2} \right) \frac{k_B T}{\pi} \right]^{1/2} \frac{k_B T}{P} \frac{1 + \Delta_{12}}{\sigma_{12}^2 \Omega_{12}^{(1,1)*}(T_{12}^*)}, \quad (5)$$

where m_1 and m_2 are the mass of the molecules, $\Omega_{12}^{(1,1)*}(T_{12}^*)$ and $\Omega_{12}^{(2,2)*}(T_{12}^*)$ are the reduced diffusion and viscosity collision integrals for binary mixture as a function of reduced temperature $T_{12}^*(\equiv k_B T / \varepsilon_{12})$, f_η and Δ_{12} are the higher-order correction factors of interaction viscosity and binary diffusion, respectively, which can be defined as

$$f_\eta = 1 + \frac{3}{196} (6E_{12}^* - 7)^2, \quad (6)$$

$$\Delta_{12} \approx 1.3(6C_{12}^* - 5)^2 \frac{a_{12}x_1}{1 + b_{12}x_1}, \quad (7)$$

where x_1 and x_2 are mole fractions of species 1 and 2, respectively, and C_{12}^* and E_{12}^* are the ratio collision integrals, which are defined as

$$C_{12}^* \equiv \frac{\Omega_{12}^{(1,2)*}}{\Omega_{12}^{(1,1)*}}, \quad (8)$$

$$E_{12}^* \equiv \frac{\Omega_{12}^{(2,3)*}}{\Omega_{12}^{(2,2)*}}, \quad (9)$$

and

$$a_{12} = \frac{\sqrt{2}}{8[1 + 1.8(m_2/m_1)]^2} \frac{\Omega_{12}^{(1,1)*}(T_{12}^*)}{\Omega_{12}^{(2,2)*}(T_{12}^*)} \quad (10)$$

$$b_{12} = 10a_{12}[1 + 1.8(m_2/m_1) + 3(m_2/m_1)^2] - 1. \quad (11)$$

The value of f_η differs from unity by only 1%, and can be determined from the ratio collision integral E_{12}^* . Numerical differentiation and use of the following recursion relation can generate collision integrals higher than that mentioned

$$\Omega^{(l,s+1)*} = \Omega^{(l,s)*} \left[1 + \left(\frac{1}{s} + 2 \right) \frac{d \ln \Omega^{(l,s)*}}{d \ln T^*} \right], \quad (12)$$

where the reduced collision integral $\Omega^{(l,s)*}$ is defined as

$$\Omega^{(l,s)*} = \frac{\Omega^{(l,s)}}{\pi \sigma^2}. \quad (13)$$

Intermolecular Potential of Non-Spherical Molecules.

The attractive energy of two non-spherical molecules is normally divided into the interaction between permanent electrostatic distributions (dipoles and possibly higher-multipoles) and interactions involving electric moments induced by the permanent moments of other molecules.¹⁹ Molecules a and b of species 1 and 2 can be assumed to have arbitrary charge distributions with 2^n -pole and 2^m -pole electric moments, respectively. In the case of non-overlapping charge distributions, molecules a and b, which are separated by distance r_{ab} and have orientations specified by ω_a and ω_b , have an electrostatic potential energy u_{12}^{el} given by the following expansion:

$$u_{12}^{\text{el}}(r_{ab}, \omega_a, \omega_b) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^{m+1} 2^{n+m} n! m!}{(2n)!(2m)!} \times \mathbf{M}_{a1}^{(n)}[n] \mathbf{T}_{ab}^{(m)}[m] \mathbf{M}_{b2}, \quad (14)$$

where

$${}^{(n)}\mathbf{T}_{ab}^{(m)} \equiv -\nabla^{n+m} \left(\frac{1}{r_{ab}} \right) \quad a \neq b, \quad (15)$$

is a tensor of rank $n + m$ describing the (2^n -pole)–(2^m -pole) interactions between the molecules a and b, and ∇ is directed from molecule a to b.

Moreover, to within the induced-dipole approximation, the induction potential energy of two unlike molecules is given by

$$u_{12}^{\text{ind}}(r_{ab}, \omega_a, \omega_b) = -\frac{1}{2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^{m+1} 2^{n+m} n! m!}{(2n)!(2m)!} \times \left\{ \begin{aligned} &\mathbf{M}_{a1}^{(n)}[n] {}^{(n)}\mathbf{T}_{ab}^{(1)} \cdot \boldsymbol{\alpha}_{b2} \cdot {}^{(1)}\mathbf{T}_{ba}^{(m)}[m] \mathbf{M}_{a1} \\ &+ \mathbf{M}_{b2}^{(m)}[m] {}^{(n)}\mathbf{T}_{ba}^{(1)} \cdot \boldsymbol{\alpha}_{a1} \cdot {}^{(1)}\mathbf{T}_{ab}^{(m)}[m] \mathbf{M}_{b2} \end{aligned} \right\}, \quad (16)$$

where $\boldsymbol{\alpha}_i$ is the electric dipole polarizability tensor of molecule λ ($\lambda = a, b$) of species i ($i = 1, 2$), α_i is the scalar dipole polarizability of species i , and $\mathbf{M}_{a1}^{(n)}$ is the n th rank tensor of the electric multipole moment (monopole, dipole, quadrupole, octapole, etc.) of molecule a of species 1, which can be written as:

$$\mathbf{M}^{(0)} = \sum_{\lambda} q_{\lambda 1} \equiv q, \quad (17a)$$

$$\mathbf{M}^{(1)} = \sum_{\lambda} q_{\lambda 1} \mathbf{r}_{\lambda 1} \equiv \boldsymbol{\mu}, \quad (17b)$$

$$\mathbf{M}^{(2)} = \frac{1}{2} \sum_{\lambda} q_{\lambda 1} (3\mathbf{r}_{\lambda 1} \mathbf{r}_{\lambda 1} - r_{\lambda 1}^2 \mathbf{U}_{12}) \equiv \boldsymbol{\Theta}, \quad (17c)$$

$$\mathbf{M}^{(3)} = \frac{1}{2} \sum_{\lambda} q_{\lambda 1} \{ 5\mathbf{r}_{\lambda 1} \mathbf{r}_{\lambda 1} \mathbf{r}_{\lambda 1} - r_{\lambda 1}^2 (\mathbf{U}_{12} \mathbf{r}_{\lambda 1} + \mathbf{U}_{23} \mathbf{r}_{\lambda 1} + \mathbf{U}_{31} \mathbf{r}_{\lambda 2}) \} \equiv \boldsymbol{\Omega}, \quad (17d)$$

where q , $\boldsymbol{\mu}$, $\boldsymbol{\Theta}$, and $\boldsymbol{\Omega}$ are the monopole, dipole, quadrupole, and octapole of molecule a of species 1, respectively (for simplicity we have dropped a and 1), $q_{\lambda 1}$ is the electric charge of molecule λ of species 1 and \mathbf{U}_{ij} is a unit tensor.

Non-Spherical Contributions to Collision Integrals. We used perturbation expansion to treat the directional component as a perturbation on the spherical field. To do so, we presented that the perturbation was applied gradually, giving a continuous change from the unperturbed (Lennard–Jones potential) to the perturbed (directional part of intermolecular potential) system. Mathematically, this corresponds to introducing a perturbation parameter ζ into the potential, so that

$$u^*(r, \omega_1, \omega_2) = u_0^*(r) + \zeta u_{ns}^*(r, \omega_1, \omega_2). \quad (18)$$

The scattering angle (χ) and the reduced cross section $Q^{*(l)}$ were then expanded as Taylor series in powers of ζ :

$$\chi(b^*, E^*, \zeta) = \chi_0(b^*, E^*) + \zeta \chi_1(b^*, E^*) + \zeta^2 \chi_2(b^*, E^*) + \dots \quad (19)$$

$$Q^{(l)*}(E^*, \zeta) = Q_0^{(l)*}(E^*) + \zeta Q_1^{(l)*}(E^*) + \zeta^2 Q_2^{(l)*}(E^*) + \dots \quad (20)$$

Substituting Eqs. 19 and 20 into Eqs. 1 and 2, collecting like powers of ζ and equating the coefficients of ζ^n terms, we then have

$$\chi_0(b^*, E^*) = \pi - 2b^* \int_0^\infty \frac{r^{*-2} dr^*}{\{1 - (b^{*2}/r^{*2}) - [u_0^*(r^*)/E^*]\}^{1/2}}, \quad (21)$$

$$\chi_1(b^*, E^*) = -\frac{b^*}{E^*} \iint d\omega_a d\omega_b \int_0^\infty [u_{ns}^*(r^*, \omega_a, \omega_b)] \times \frac{r^{*-2} dr^*}{\{1 - (b^{*2}/r^{*2}) - [u_0^*(r^*)/E^*]\}^{3/2}}, \quad (22)$$

$$\chi_2(b^*, E^*) = -\frac{3}{2} \frac{b^*}{E^{*2}} \iint d\omega_a d\omega_b \int_0^\infty [u_{ns}^*(r^*, \omega_a, \omega_b)]^2 \times \frac{r^{*-2} dr^*}{\{1 - (b^{*2}/r^{*2}) - [u_0^*(r^*)/E^*]\}^{5/2}}, \quad (23)$$

and

$$Q_0^{(l)*}(E^*) = 2 \left[1 - \frac{1 + (-1)^l}{2(1+l)} \right]^{-1} \times \int_0^\infty (1 - \cos^l \chi_0) b^* db^*, \quad (24)$$

$$Q_1^{(l)*}(E^*) = 2l \left[1 - \frac{1 + (-1)^l}{2(1+l)} \right]^{-1} \times \int_0^\infty [\chi_1 \sin \chi_0 \cos^{l-1} \chi_0] b^* db^*, \quad (25)$$

$$Q_2^{(l)*}(E^*) = 2 \left[1 - \frac{1 + (-1)^l}{2(1+l)} \right]^{-1} \times \int_0^\infty [l\chi_1^2 \cos^l \chi_0 + l\chi_2 \sin \chi_0 \cos^{l-1} \chi_0 + l(l-1)\chi_1^2 \sin^2 \chi_0 \cos^{l-2} \chi_0] b^* db^*, \quad (26)$$

where

$$u_0^*(r^*) = 4 \left[\left(\frac{1}{r^*} \right)^{12} - \left(\frac{1}{r^*} \right)^6 \right], \quad (27)$$

and

$$u_{ns}^*(r^*, \omega_1, \omega_2) = u_{el}^*(r^*, \omega_1, \omega_2) + u_{ind}^*(r^*, \omega_1, \omega_2), \quad (28)$$

where $u_{el}^*(r^*, \omega_1, \omega_2)$ and $u_{ind}^*(r^*, \omega_1, \omega_2)$ are defined in Eqs. 14 and 16, respectively.

Electrostatic Contribution to χ : In the first approximation, electrostatic interactions of permanent multipoles do not contribute to the χ (Eq. 22), because the first power of $u_{el}^*(r^*, \omega_1, \omega_2)$ vanishes on isotropic averaging, i.e., on integration over all possible orientations of the molecules with equal probability. The first nonzero contribution to χ comes in the second approximation from the square of $u_{el}^*(r^*, \omega_1, \omega_2)$, Eq. 23. By substituting Eq. 14 into Eq. 23 and carrying out integration over all orientation coordinates, we obtained

$$\chi_{2,el}^* = -\frac{3(4\pi)^2 b^*}{2E^{*2}} \sum_{n=0}^\infty \sum_{m=0}^\infty \frac{2^{(n+m)} (n!m!)^2 (2n+2m)!}{(2n)!(2m)!(2n+1)!(2m+1)!} \times (M_1^{*(n)} [n]^{(n)} M_1^*) (M_2^{*(m)} [m]^{(m)} M_2^*) \times Z[2(n+m+1), 2], \quad (29)$$

where $M_i^{*(n)}$ is the n th rank tensor of the reduced electric multipole moment, and

$$Z[k, l] \equiv \int_0^\infty \frac{r^{*-2} dr^*}{\{1 - (b^{*2}/r^{*2}) - [u_0^*(r^*)/E^*]\}^{1/2}} \times \frac{r^{*-k}}{\{1 - (b^{*2}/r^{*2}) - [u_0^*(r^*)/E^*]\}^l}. \quad (30)$$

Induction Contribution to χ : The first-order contribution to the scattering angle from the induced-dipole interaction can be obtained by substituting Eq. 16 into 22 and carrying out integration over all orientation coordinates, affording:

$$\chi_{1,ind}^* = -\frac{(2\pi)^2 b^*}{E^*} \sum_{n=0}^\infty \frac{2^n (2n+2)! (n!)^2}{(2n)!(2n+1)!} \{ \alpha_1 (M_1^{(n)} [n]^{(n)} M_1) + (M_2^{(n)} n^{(n)} M_2) \alpha_2 \} Z[2(n+2), 1]. \quad (31)$$

Cross Contributions to χ : A further contribution to χ within the second-order approximation can be obtained from the cross term $u_{el}^* u_{ind}^*$. For a case with isotropic dipole polarizability α , this cross term vanishes by averaging over all orientations, but for cases with anisotropic polarizability α . If the molecule possesses dipole or quadrupole moments, the cross term $u_{el}^* u_{ind}^*$ is nonzero, and $\chi_{2,cross}(b^*, E^*)$ can be written as:

$$\chi_{2,cross}^*(b^*, E^*) = \frac{3b^*}{E^{*2}} \left\{ \frac{4(4\pi)^2}{5} [(\alpha_1^* : \Theta_1^*)(\mu_2^* \cdot \Theta_2^* \cdot \mu_2^*) + (\mu_1^* \cdot \Theta_1^* \cdot \mu_1^*)(\alpha_2^* : \Theta_2^*)] Z[13, 2] + \frac{16(4\pi)^2}{35} [(\alpha_1^* : \Theta_1^*)(\Theta_2^* : (\Theta_2^* \cdot \Theta_2^*)) + (\Theta_1^* : (\Theta_1^* \cdot \Theta_1^*))(\alpha_2^* : \Theta_2^*)] Z[15, 2] \right\}, \quad (32)$$

where the reduced dipole moment μ_i^* , reduced quadrupole moment Θ_i^* , and reduced dipole polarizability α_i^* are defined as:

$$\mu_i^* \equiv \frac{\mu_i}{(\epsilon \sigma^3)^{1/2}}, \quad (33a)$$

$$\Theta_i^* \equiv \frac{\Theta_i}{(\epsilon \sigma^5)^{1/2}}, \quad (33b)$$

$$\alpha_i^* \equiv \frac{\alpha_i}{\sigma^3}. \quad (33c)$$

Results and Discussion

In this work, we obtained the general expressions for non-spherical contributions to the collision integrals, which are Eqs. 29–32. These expressions are valid in general for molecules of arbitrary symmetry and arbitrary electronic structure.¹⁹ The expressions are applied to cases of axially symmetric with respect to the z -axis, in which $M_{ai}^{(n)}$ is the scalar multipole moment of order n :

$$M_k^{(n)} [n] M_k^{(n)} = \frac{(2n)!}{2^n (n!)^2} (M_k^{(n)})^2 \quad (34)$$

Table 1. Spherical Contribution to the Reduced Collision Integrals

| T^* | $\Omega_0^{(1,1)*}$ | $\Omega_0^{(1,2)*}$ | $\Omega_0^{(1,3)*}$ | $\Omega_0^{(2,2)*}$ | $\Omega_0^{(2,3)*}$ |
|-------|---------------------|---------------------|---------------------|---------------------|---------------------|
| 1.0 | 1.4391 | 1.2040 | 1.0761 | 1.3896 | 1.3091 |
| 1.2 | 1.3200 | 1.1191 | 1.0136 | 1.2812 | 1.2112 |
| 1.4 | 1.2333 | 1.0591 | 0.9694 | 1.2051 | 1.1413 |
| 1.6 | 1.1678 | 1.0143 | 0.9361 | 1.1492 | 1.0893 |
| 1.8 | 1.1165 | 0.9795 | 0.9098 | 1.1063 | 1.0490 |
| 2.0 | 1.0753 | 0.9516 | 0.8884 | 1.0724 | 1.0168 |
| 2.5 | 1.0007 | 0.9004 | 0.8483 | 1.0117 | 0.9589 |
| 3.0 | 0.9501 | 0.8649 | 0.8195 | 0.9708 | 0.9195 |
| 3.5 | 0.9132 | 0.8383 | 0.7972 | 0.9408 | 0.8905 |
| 4.0 | 0.8847 | 0.8172 | 0.7791 | 0.9174 | 0.8679 |
| 4.5 | 0.8618 | 0.7998 | 0.7639 | 0.8984 | 0.8494 |
| 5.0 | 0.8429 | 0.7850 | 0.7508 | 0.8824 | 0.8340 |
| 5.5 | 0.8268 | 0.7722 | 0.7394 | 0.8687 | 0.8207 |
| 6.0 | 0.8129 | 0.7610 | 0.7292 | 0.8567 | 0.8090 |
| 6.5 | 0.8007 | 0.7510 | 0.7200 | 0.8460 | 0.7987 |
| 7.0 | 0.7899 | 0.7419 | 0.7117 | 0.8364 | 0.7894 |
| 7.5 | 0.7801 | 0.7337 | 0.7041 | 0.8276 | 0.7809 |
| 8.0 | 0.7712 | 0.7261 | 0.6971 | 0.8196 | 0.7732 |
| 8.5 | 0.7631 | 0.7191 | 0.6905 | 0.8122 | 0.7661 |
| 9.0 | 0.7557 | 0.7126 | 0.6845 | 0.8053 | 0.7594 |
| 9.5 | 0.7488 | 0.7066 | 0.6788 | 0.7989 | 0.7533 |
| 10.0 | 0.7423 | 0.7009 | 0.6734 | 0.7929 | 0.7475 |
| 12.0 | 0.7203 | 0.6812 | 0.6548 | 0.7720 | 0.7274 |
| 14.0 | 0.7026 | 0.6652 | 0.6394 | 0.7549 | 0.7110 |
| 16.0 | 0.6879 | 0.6515 | 0.6263 | 0.7402 | 0.6969 |
| 18.0 | 0.6752 | 0.6397 | 0.6146 | 0.7271 | 0.6844 |
| 20.0 | 0.6640 | 0.6290 | 0.6037 | 0.7148 | 0.6727 |

Table 2. Values for Molecular Parameters Used in Evaluation of Non-Spherical Contribution to the Collision Integrals

| | $\varepsilon/k_B/K$ | $\sigma/\text{\AA}$ | μ^* | Θ^* | α^* |
|----|---------------------|---------------------|---------|------------|------------|
| NO | 119.5 | 3.425 | 0.188 | 0.646 | 0.0462 |
| CO | 110.0 | 3.590 | 0.134 | 0.829 | 0.0425 |

where $M_k^{(n)}$ is the scalar multipole moment of order n for the axially symmetry molecule of species k . Therefore, in the case of a pure gas consisting of axially symmetric molecules, such as NO and CO, μ and Θ , the expressions for electrostatic contributions to χ and the reduced cross section $Q^{*(l)}$ could be obtained in terms of molecular parameters.

Moreover, in case of calculating the inductive contribution, we implicitly assumed that the polarizabilities of the molecules were isotropic so that the electric dipole polarizability tensors were scalar quantities. In case of induction interaction, our treatment was valid within the induced dipole approximation, and the contribution due to higher-order induced moments and hyperpolarizabilities was not included. Clearly, for these molecules, the cross contribution $\chi_{2,\text{cross}}^*$ vanished by averaging over all orientations. The results were then applied to the evaluation of the collision integrals of NO and CO. Table 1 shows the spherical contribution to the reduced collision integrals $\Omega_0^{(l,s)*}$ as a function of reduced temperature T^* .

The values for the molecular parameters used in evaluation of non-spherical contribution to the collision integrals are given in Table 2. The experimental values of μ and Θ and dipole

polarizability were taken from Refs. 20, 21, and 22, respectively. The values of the scaling potential parameters σ and ε/k_B were obtained from experimental viscosity data at two arbitrary temperatures, T_1 and T_2 . For this purpose, we first defined the quantity K_η as

$$K_\eta = \left[\frac{\eta(T_2)}{\eta(T_1)} \right]_{\text{exp}} \left(\frac{T_1}{T_2} \right)^{1/2}. \quad (35)$$

Using Eq. 4, we obtained an alternative equation in terms of T^* :

$$K_\eta = \left[\frac{\Omega^{(2,2)*}(T_1^*)}{\Omega^{(2,2)*}(T_2^*)} \right] \left[\frac{f_\eta(T_2^*)}{f_\eta(T_1^*)} \right], \quad (36)$$

where the reduced temperature (T_i^*) relates to ε/k_B as

$$T_i^* = \frac{k_B T_i}{\varepsilon}. \quad (37)$$

Here, $f_\eta(T^*)$ was defined in Eq. 6. By employing the experimental points of (η, T) , the experimental value of K_η was obtained from Eq. 35. Making an initial guess at the potential well depth that is denoted as ε_0 , the initial estimates of data points ($\Omega^{(2,2)*}, T^*$) and (f_η, T^*) could be obtained at T_1 and T_2 . As a first approximation to ε/k_B , the value calculated from the critical temperature¹⁸ as $\varepsilon_0/k_B = 0.77T_c$, where T_c is the critical temperature, was used. We then generated the approximate value of K_η from Eq. 36 and compared it with the observed value of K_η obtained from Eq. 35. We used repeated trials to establish the minimum deviation between the observed value of ε/k_B , based on Eq. 35, and the calculated value of ε/k_B , obtained from Eq. 36. Once the value of ε/k_B was determined, the parameter σ was obtained from:

$$\sigma = \left\{ \frac{266.93 \sqrt{m T_i} f_\eta(T_i^*)}{[\eta(T_i) \times 10^7] \Omega^{(2,2)*}(T_i^*)} \right\}^{1/2}, \quad (38)$$

where T_i is either T_1 or T_2 . The values of σ and ε/k_B are also given in Table 2.

The integrals involved in computing $\Omega_{ns}^{(l,s)*}$ could not be solved analytically and therefore, were solved by using numerical methods. The procedure reported by Barker et al.²² was used in this work. The results are shown in Tables 3–7. As can be seen from the Tables, each term in the non-spherical part of the potential had a definite contribution to the collision integrals. The maximum effects on the nonspherical contribution to both $\Omega^{(1,1)}$ and $\Omega^{(2,2)}$ of CO and NO came from the dipole–dipole and dipole–quadrupole terms. Figure 1 shows the electrostatic and inductive contributions to the $\Omega^{(l,s)*}$ of CO and NO as a function of T^* .

Figures 2 and 3 show the deviation percent between the calculated and experimental values²³ of η and D of CO and NO, which defined as $\frac{(Y_{\text{cal}} - Y_{\text{exp}}) \times 100}{Y_{\text{cal}}}$, where $Y \equiv \eta$ or D . The deviation in the calculated values of viscosity coefficients was less than 1% in the temperature range $200 \text{ K} < T < 1000 \text{ K}$, whereas it was 3% between our calculated values of diffusion coefficients and those experimental data.

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Table 3. Dipole–Dipole Contribution to the Reduced Collision Integrals

| T^* | CO | | | | | NO | | | | |
|-------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| | $\Omega_{dd}^{(1,1)*}$ | $\Omega_{dd}^{(1,2)*}$ | $\Omega_{dd}^{(1,3)*}$ | $\Omega_{dd}^{(2,2)*}$ | $\Omega_{dd}^{(2,3)*}$ | $\Omega_{dd}^{(1,1)*}$ | $\Omega_{dd}^{(1,2)*}$ | $\Omega_{dd}^{(1,3)*}$ | $\Omega_{dd}^{(2,2)*}$ | $\Omega_{dd}^{(2,3)*}$ |
| 1.0 | 0.0694 | 0.0624 | 0.0576 | −0.2120 | −0.1940 | 0.0719 | 0.0615 | 0.0553 | −0.1966 | −0.1779 |
| 1.2 | 0.0656 | 0.0588 | 0.0537 | −0.2014 | −0.1899 | 0.0665 | 0.0571 | 0.0513 | −0.1858 | −0.1741 |
| 1.4 | 0.0624 | 0.0555 | 0.0502 | −0.1951 | −0.1854 | 0.0623 | 0.0536 | 0.0479 | −0.1795 | −0.1701 |
| 1.6 | 0.0597 | 0.0526 | 0.0472 | −0.1896 | −0.1784 | 0.0589 | 0.0505 | 0.0449 | −0.1743 | −0.1637 |
| 1.8 | 0.0572 | 0.0501 | 0.0445 | −0.1836 | −0.1691 | 0.0560 | 0.0479 | 0.0423 | −0.1687 | −0.1553 |
| 2.0 | 0.0549 | 0.0477 | 0.0422 | −0.1767 | −0.1586 | 0.0535 | 0.0455 | 0.0399 | −0.1624 | −0.1458 |
| 2.5 | 0.0501 | 0.0429 | 0.0375 | −0.1571 | −0.1315 | 0.0482 | 0.0406 | 0.0352 | −0.1444 | −0.1210 |
| 3.0 | 0.0462 | 0.0391 | 0.0340 | −0.1368 | −0.1073 | 0.0441 | 0.0368 | 0.0318 | −0.1259 | −0.0988 |
| 3.5 | 0.0429 | 0.0361 | 0.0314 | −0.1182 | −0.0875 | 0.0408 | 0.0339 | 0.0293 | −0.1088 | −0.0806 |
| 4.0 | 0.0402 | 0.0337 | 0.0294 | −0.1019 | −0.0719 | 0.0381 | 0.0315 | 0.0273 | −0.0938 | −0.0662 |
| 4.5 | 0.0380 | 0.0317 | 0.0277 | −0.0881 | −0.0597 | 0.0358 | 0.0296 | 0.0257 | −0.0811 | −0.0550 |
| 5.0 | 0.0360 | 0.0301 | 0.0263 | −0.0765 | −0.0502 | 0.0339 | 0.0280 | 0.0244 | −0.0705 | −0.0463 |
| 5.5 | 0.0344 | 0.0287 | 0.0252 | −0.0669 | −0.0429 | 0.0323 | 0.0267 | 0.0234 | −0.0617 | −0.0395 |
| 6.0 | 0.0329 | 0.0275 | 0.0243 | −0.0590 | −0.0373 | 0.0309 | 0.0256 | 0.0225 | −0.0543 | −0.0342 |
| 6.5 | 0.0317 | 0.0266 | 0.0236 | −0.0524 | −0.0330 | 0.0296 | 0.0246 | 0.0217 | −0.0482 | −0.0301 |
| 7.0 | 0.0306 | 0.0257 | 0.0231 | −0.0470 | −0.0297 | 0.0285 | 0.0238 | 0.0209 | −0.0431 | −0.0267 |
| 7.5 | 0.0296 | 0.0250 | 0.0227 | −0.0425 | −0.0273 | 0.0276 | 0.0230 | 0.0200 | −0.0388 | −0.0240 |
| 8.0 | 0.0287 | 0.0245 | 0.0223 | −0.0388 | −0.0256 | 0.0267 | 0.0222 | 0.0190 | −0.0351 | −0.0215 |
| 8.5 | 0.0280 | 0.0240 | 0.0220 | −0.0358 | −0.0244 | 0.0259 | 0.0214 | 0.0178 | −0.0319 | −0.0192 |
| 9.0 | 0.0273 | 0.0235 | 0.0216 | −0.0334 | −0.0235 | 0.0251 | 0.0205 | 0.0163 | −0.0291 | −0.0169 |
| 9.5 | 0.0267 | 0.0231 | 0.0213 | −0.0314 | −0.0229 | 0.0243 | 0.0195 | 0.0146 | −0.0265 | −0.0145 |
| 10.0 | 0.0262 | 0.0227 | 0.0209 | −0.0298 | −0.0225 | 0.0236 | 0.0184 | 0.0125 | −0.0240 | −0.0119 |
| 12.0 | 0.0244 | 0.0211 | 0.0184 | −0.0255 | −0.0203 | 0.0202 | 0.0125 | 0.0020 | −0.0144 | 0.0006 |
| 14.0 | 0.0228 | 0.0190 | 0.0144 | −0.0222 | −0.0163 | 0.0159 | 0.0047 | −0.0102 | −0.0038 | 0.0154 |
| 16.0 | 0.0210 | 0.0160 | 0.0091 | −0.0185 | −0.0102 | 0.0107 | −0.0041 | −0.0218 | 0.0073 | 0.0297 |
| 18.0 | 0.0190 | 0.0122 | 0.0031 | −0.0139 | −0.0028 | 0.0049 | −0.0128 | −0.0316 | 0.0182 | 0.0418 |
| 20.0 | 0.0165 | 0.0080 | −0.0029 | −0.0087 | 0.0047 | −0.0010 | −0.0207 | −0.0396 | 0.0281 | 0.0515 |

Table 4. Dipole–Quadrupole Contribution to the Reduced Collision Integrals

| T^* | CO | | | | | NO | | | | |
|-------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| | $\Omega_{dq}^{(1,1)*}$ | $\Omega_{dq}^{(1,2)*}$ | $\Omega_{dq}^{(1,3)*}$ | $\Omega_{dq}^{(2,2)*}$ | $\Omega_{dq}^{(2,3)*}$ | $\Omega_{dq}^{(1,1)*}$ | $\Omega_{dq}^{(1,2)*}$ | $\Omega_{dq}^{(1,3)*}$ | $\Omega_{dq}^{(2,2)*}$ | $\Omega_{dq}^{(2,3)*}$ |
| 1.0 | 0.0337 | 0.0257 | 0.0281 | −0.1461 | −0.1472 | 0.0961 | 0.0799 | 0.0635 | −0.2152 | −0.1933 |
| 1.2 | 0.0307 | 0.0271 | 0.0286 | −0.1487 | −0.1538 | 0.0864 | 0.0671 | 0.0493 | −0.1993 | −0.1782 |
| 1.4 | 0.0295 | 0.0279 | 0.0294 | −0.1520 | −0.1570 | 0.0771 | 0.0566 | 0.0409 | −0.1869 | −0.1679 |
| 1.6 | 0.0292 | 0.0289 | 0.0312 | −0.1542 | −0.1570 | 0.0690 | 0.0493 | 0.0376 | −0.1773 | −0.1601 |
| 1.8 | 0.0293 | 0.0303 | 0.0340 | −0.1548 | −0.1545 | 0.0624 | 0.0448 | 0.0374 | −0.1695 | −0.1537 |
| 2.0 | 0.0298 | 0.0321 | 0.0371 | −0.1540 | −0.1506 | 0.0572 | 0.0425 | 0.0391 | −0.1630 | −0.1479 |
| 2.5 | 0.0323 | 0.0374 | 0.0437 | −0.1478 | −0.1372 | 0.0498 | 0.0424 | 0.0448 | −0.1496 | −0.1341 |
| 3.0 | 0.0355 | 0.0416 | 0.0466 | −0.1379 | −0.1212 | 0.0472 | 0.0446 | 0.0478 | −0.1374 | −0.1191 |
| 3.5 | 0.0383 | 0.0439 | 0.0461 | −0.1261 | −0.1047 | 0.0466 | 0.0461 | 0.0473 | −0.1251 | −0.1035 |
| 4.0 | 0.0402 | 0.0443 | 0.0437 | −0.1138 | −0.0893 | 0.0464 | 0.0460 | 0.0446 | −0.1128 | −0.0886 |
| 4.5 | 0.0413 | 0.0434 | 0.0404 | −0.1018 | −0.0758 | 0.0462 | 0.0448 | 0.0410 | −0.1011 | −0.0754 |
| 5.0 | 0.0417 | 0.0418 | 0.0369 | −0.0907 | −0.0644 | 0.0455 | 0.0428 | 0.0371 | −0.0901 | −0.0640 |
| 5.5 | 0.0414 | 0.0397 | 0.0336 | −0.0808 | −0.0549 | 0.0445 | 0.0404 | 0.0335 | −0.0802 | −0.0545 |
| 6.0 | 0.0408 | 0.0374 | 0.0307 | −0.0720 | −0.0473 | 0.0433 | 0.0378 | 0.0302 | −0.0714 | −0.0467 |
| 6.5 | 0.0398 | 0.0352 | 0.0283 | −0.0643 | −0.0412 | 0.0418 | 0.0354 | 0.0275 | −0.0637 | −0.0405 |
| 7.0 | 0.0387 | 0.0332 | 0.0262 | −0.0577 | −0.0365 | 0.0403 | 0.0330 | 0.0251 | −0.0571 | −0.0357 |
| 7.5 | 0.0375 | 0.0313 | 0.0246 | −0.0521 | −0.0330 | 0.0387 | 0.0309 | 0.0232 | −0.0515 | −0.0320 |
| 8.0 | 0.0362 | 0.0296 | 0.0232 | −0.0475 | −0.0304 | 0.0372 | 0.0289 | 0.0217 | −0.0467 | −0.0294 |
| 8.5 | 0.0350 | 0.0281 | 0.0222 | −0.0436 | −0.0287 | 0.0357 | 0.0272 | 0.0204 | −0.0428 | −0.0275 |
| 9.0 | 0.0338 | 0.0268 | 0.0213 | −0.0404 | −0.0275 | 0.0342 | 0.0257 | 0.0194 | −0.0395 | −0.0262 |
| 9.5 | 0.0327 | 0.0257 | 0.0206 | −0.0378 | −0.0268 | 0.0328 | 0.0244 | 0.0186 | −0.0368 | −0.0254 |
| 10.0 | 0.0316 | 0.0247 | 0.0201 | −0.0358 | −0.0265 | 0.0315 | 0.0233 | 0.0180 | −0.0347 | −0.0250 |
| 12.0 | 0.0280 | 0.0219 | 0.0188 | −0.0309 | −0.0266 | 0.0273 | 0.0200 | 0.0164 | −0.0296 | −0.0249 |
| 14.0 | 0.0254 | 0.0203 | 0.0180 | −0.0290 | −0.0267 | 0.0242 | 0.0182 | 0.0156 | −0.0274 | −0.0249 |
| 16.0 | 0.0235 | 0.0192 | 0.0172 | −0.0279 | −0.0259 | 0.0220 | 0.0169 | 0.0149 | −0.0262 | −0.0241 |
| 18.0 | 0.0221 | 0.0183 | 0.0163 | −0.0268 | −0.0242 | 0.0203 | 0.0160 | 0.0141 | −0.0252 | −0.0226 |
| 20.0 | 0.0209 | 0.0174 | 0.0154 | −0.0256 | −0.0221 | 0.0190 | 0.0152 | 0.0133 | −0.0239 | −0.0207 |

Table 5. Quadrupole–Quadrupole Contribution to the Reduced Collision Integrals

| T^* | CO | | | | | NO | | | | |
|-------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| | $\Omega_{qq}^{(1,1)*}$ | $\Omega_{qq}^{(1,2)*}$ | $\Omega_{qq}^{(1,3)*}$ | $\Omega_{qq}^{(2,2)*}$ | $\Omega_{qq}^{(2,3)*}$ | $\Omega_{qq}^{(1,1)*}$ | $\Omega_{qq}^{(1,2)*}$ | $\Omega_{qq}^{(1,3)*}$ | $\Omega_{qq}^{(2,2)*}$ | $\Omega_{qq}^{(2,3)*}$ |
| 1.0 | 0.0179 | 0.0099 | 0.0063 | 0.0282 | 0.0180 | 0.0195 | 0.0130 | 0.0117 | 0.0320 | 0.0274 |
| 1.2 | 0.0140 | 0.0076 | 0.0049 | 0.0218 | 0.0142 | 0.0166 | 0.0126 | 0.0127 | 0.0297 | 0.0277 |
| 1.4 | 0.0113 | 0.0062 | 0.0042 | 0.0176 | 0.0116 | 0.0152 | 0.0130 | 0.0143 | 0.0291 | 0.0290 |
| 1.6 | 0.0095 | 0.0053 | 0.0038 | 0.0147 | 0.0097 | 0.0146 | 0.0140 | 0.0163 | 0.0294 | 0.0309 |
| 1.8 | 0.0081 | 0.0047 | 0.0038 | 0.0125 | 0.0082 | 0.0146 | 0.0153 | 0.0185 | 0.0303 | 0.0327 |
| 2.0 | 0.0072 | 0.0044 | 0.0038 | 0.0108 | 0.0069 | 0.0150 | 0.0167 | 0.0204 | 0.0314 | 0.0339 |
| 2.5 | 0.0057 | 0.0041 | 0.0040 | 0.0076 | 0.0042 | 0.0167 | 0.0198 | 0.0226 | 0.0329 | 0.0330 |
| 3.0 | 0.0050 | 0.0041 | 0.0039 | 0.0052 | 0.0021 | 0.0183 | 0.0209 | 0.0209 | 0.0313 | 0.0266 |
| 3.5 | 0.0046 | 0.0039 | 0.0033 | 0.0033 | 0.0000 | 0.0192 | 0.0200 | 0.0170 | 0.0269 | 0.0176 |
| 4.0 | 0.0043 | 0.0035 | 0.0025 | 0.0015 | −0.0020 | 0.0191 | 0.0178 | 0.0126 | 0.0211 | 0.0088 |
| 4.5 | 0.0040 | 0.0029 | 0.0016 | −0.0002 | −0.0039 | 0.0183 | 0.0150 | 0.0087 | 0.0150 | 0.0017 |
| 5.0 | 0.0036 | 0.0023 | 0.0008 | −0.0018 | −0.0053 | 0.0170 | 0.0123 | 0.0058 | 0.0095 | −0.0032 |
| 5.5 | 0.0032 | 0.0017 | 0.0002 | −0.0030 | −0.0061 | 0.0155 | 0.0099 | 0.0040 | 0.0050 | −0.0059 |
| 6.0 | 0.0028 | 0.0012 | 0.0000 | −0.0040 | −0.0062 | 0.0140 | 0.0080 | 0.0031 | 0.0016 | −0.0068 |
| 6.5 | 0.0024 | 0.0009 | 0.0001 | −0.0045 | −0.0057 | 0.0125 | 0.0066 | 0.0030 | −0.0006 | −0.0062 |
| 7.0 | 0.0021 | 0.0007 | 0.0003 | −0.0047 | −0.0047 | 0.0113 | 0.0058 | 0.0035 | −0.0019 | −0.0045 |
| 7.5 | 0.0018 | 0.0007 | 0.0007 | −0.0045 | −0.0034 | 0.0102 | 0.0053 | 0.0044 | −0.0022 | −0.0021 |
| 8.0 | 0.0016 | 0.0007 | 0.0012 | −0.0041 | −0.0018 | 0.0093 | 0.0052 | 0.0055 | −0.0018 | 0.0008 |
| 8.5 | 0.0015 | 0.0009 | 0.0018 | −0.0034 | −0.0002 | 0.0087 | 0.0054 | 0.0068 | −0.0009 | 0.0038 |
| 9.0 | 0.0014 | 0.0011 | 0.0024 | −0.0026 | 0.0015 | 0.0082 | 0.0059 | 0.0081 | 0.0004 | 0.0069 |
| 9.5 | 0.0014 | 0.0014 | 0.0030 | −0.0016 | 0.0032 | 0.0079 | 0.0064 | 0.0093 | 0.0019 | 0.0098 |
| 10.0 | 0.0014 | 0.0018 | 0.0035 | −0.0005 | 0.0049 | 0.0077 | 0.0071 | 0.0105 | 0.0037 | 0.0126 |
| 12.0 | 0.0019 | 0.0033 | 0.0057 | 0.0041 | 0.0111 | 0.0081 | 0.0099 | 0.0139 | 0.0109 | 0.0213 |
| 14.0 | 0.0027 | 0.0049 | 0.0075 | 0.0087 | 0.0164 | 0.0092 | 0.0122 | 0.0155 | 0.0171 | 0.0263 |
| 16.0 | 0.0037 | 0.0063 | 0.0090 | 0.0128 | 0.0205 | 0.0105 | 0.0137 | 0.0159 | 0.0214 | 0.0286 |
| 18.0 | 0.0047 | 0.0075 | 0.0100 | 0.0163 | 0.0234 | 0.0116 | 0.0145 | 0.0156 | 0.0243 | 0.0293 |
| 20.0 | 0.0056 | 0.0085 | 0.0105 | 0.0191 | 0.0253 | 0.0124 | 0.0147 | 0.0150 | 0.0260 | 0.0291 |

Table 6. Dipole–Induced Dipole Contribution to the Reduced Collision Integrals

| T^* | CO | | | | | NO | | | | |
|-------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| | $\Omega_{d-id}^{(1,1)*}$ | $\Omega_{d-id}^{(1,2)*}$ | $\Omega_{d-id}^{(1,3)*}$ | $\Omega_{d-id}^{(2,2)*}$ | $\Omega_{d-id}^{(2,3)*}$ | $\Omega_{d-id}^{(1,1)*}$ | $\Omega_{d-id}^{(1,2)*}$ | $\Omega_{d-id}^{(1,3)*}$ | $\Omega_{d-id}^{(2,2)*}$ | $\Omega_{d-id}^{(2,3)*}$ |
| 1.0 | −0.0177 | −0.0179 | −0.0144 | 0.0244 | 0.0189 | −0.0365 | −0.0380 | −0.0307 | 0.0518 | 0.0403 |
| 1.2 | −0.0171 | −0.0148 | −0.0101 | 0.0197 | 0.0127 | −0.0357 | −0.0316 | −0.0216 | 0.0420 | 0.0270 |
| 1.4 | −0.0157 | −0.0118 | −0.0070 | 0.0153 | 0.0082 | −0.0329 | −0.0252 | −0.0149 | 0.0326 | 0.0176 |
| 1.6 | −0.0140 | −0.0093 | −0.0048 | 0.0117 | 0.0053 | −0.0294 | −0.0198 | −0.0102 | 0.0249 | 0.0112 |
| 1.8 | −0.0123 | −0.0073 | −0.0032 | 0.0088 | 0.0031 | −0.0259 | −0.0155 | −0.0068 | 0.0188 | 0.0067 |
| 2.0 | −0.0107 | −0.0057 | −0.0020 | 0.0066 | 0.0015 | −0.0226 | −0.0121 | −0.0043 | 0.0140 | 0.0033 |
| 2.5 | −0.0074 | −0.0028 | 0.0000 | 0.0025 | −0.0018 | −0.0157 | −0.0060 | 0.0001 | 0.0053 | −0.0038 |
| 3.0 | −0.0050 | −0.0009 | 0.0015 | −0.0005 | −0.0046 | −0.0107 | −0.0019 | 0.0032 | −0.0012 | −0.0100 |
| 3.5 | −0.0032 | 0.0004 | 0.0024 | −0.0029 | −0.0065 | −0.0068 | 0.0010 | 0.0054 | −0.0065 | −0.0146 |
| 4.0 | −0.0018 | 0.0014 | 0.0028 | −0.0046 | −0.0072 | −0.0038 | 0.0032 | 0.0067 | −0.0105 | −0.0173 |
| 4.5 | −0.0008 | 0.0019 | 0.0026 | −0.0055 | −0.0067 | −0.0015 | 0.0046 | 0.0071 | −0.0133 | −0.0182 |
| 5.0 | 0.0000 | 0.0021 | 0.0022 | −0.0057 | −0.0054 | 0.0003 | 0.0055 | 0.0071 | −0.0149 | −0.0179 |
| 5.5 | 0.0005 | 0.0020 | 0.0015 | −0.0053 | −0.0037 | 0.0016 | 0.0059 | 0.0068 | −0.0157 | −0.0170 |
| 6.0 | 0.0008 | 0.0017 | 0.0008 | −0.0046 | −0.0018 | 0.0026 | 0.0061 | 0.0064 | −0.0159 | −0.0158 |
| 6.5 | 0.0009 | 0.0014 | 0.0001 | −0.0035 | −0.0001 | 0.0034 | 0.0061 | 0.0059 | −0.0157 | −0.0146 |
| 7.0 | 0.0010 | 0.0010 | −0.0005 | −0.0025 | 0.0014 | 0.0039 | 0.0060 | 0.0055 | −0.0153 | −0.0136 |
| 7.5 | 0.0009 | 0.0006 | −0.0010 | −0.0014 | 0.0027 | 0.0043 | 0.0059 | 0.0052 | −0.0148 | −0.0126 |
| 8.0 | 0.0008 | 0.0002 | −0.0013 | −0.0003 | 0.0036 | 0.0046 | 0.0057 | 0.0049 | −0.0142 | −0.0118 |
| 8.5 | 0.0007 | −0.0002 | −0.0016 | 0.0006 | 0.0043 | 0.0047 | 0.0055 | 0.0046 | −0.0136 | −0.0111 |
| 9.0 | 0.0005 | −0.0005 | −0.0017 | 0.0014 | 0.0047 | 0.0048 | 0.0053 | 0.0044 | −0.0130 | −0.0105 |
| 9.5 | 0.0004 | −0.0007 | −0.0018 | 0.0021 | 0.0049 | 0.0049 | 0.0051 | 0.0042 | −0.0125 | −0.0100 |
| 10.0 | 0.0002 | −0.0009 | −0.0019 | 0.0026 | 0.0051 | 0.0049 | 0.0049 | 0.0040 | −0.0120 | −0.0095 |
| 12.0 | −0.0004 | −0.0014 | −0.0017 | 0.0038 | 0.0046 | 0.0047 | 0.0042 | 0.0033 | −0.0102 | −0.0078 |
| 14.0 | −0.0008 | −0.0014 | −0.0013 | 0.0039 | 0.0037 | 0.0044 | 0.0037 | 0.0028 | −0.0087 | −0.0063 |
| 16.0 | −0.0010 | −0.0013 | −0.0010 | 0.0036 | 0.0028 | 0.0041 | 0.0032 | 0.0022 | −0.0074 | −0.0051 |
| 18.0 | −0.0011 | −0.0011 | −0.0007 | 0.0031 | 0.0020 | 0.0038 | 0.0027 | 0.0018 | −0.0063 | −0.0040 |
| 20.0 | −0.0010 | −0.0009 | −0.0005 | 0.0027 | 0.0015 | 0.0034 | 0.0024 | 0.0015 | −0.0054 | −0.0032 |

Table 7. Cross Contribution to the Reduced Collision Integrals

| T^* | CO | | | | | NO | | | | |
|-------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|
| | $\Omega_{\text{cross}}^{(1,1)*}$ | $\Omega_{\text{cross}}^{(1,2)*}$ | $\Omega_{\text{cross}}^{(1,3)*}$ | $\Omega_{\text{cross}}^{(2,2)*}$ | $\Omega_{\text{cross}}^{(2,3)*}$ | $\Omega_{\text{cross}}^{(1,1)*}$ | $\Omega_{\text{cross}}^{(1,2)*}$ | $\Omega_{\text{cross}}^{(1,3)*}$ | $\Omega_{\text{cross}}^{(2,2)*}$ | $\Omega_{\text{cross}}^{(2,3)*}$ |
| 1.0 | 0.0121 | 0.0076 | 0.0081 | -0.0296 | -0.0273 | 0.0176 | 0.0110 | 0.0088 | 0.0173 | 0.0130 |
| 1.2 | 0.0103 | 0.0082 | 0.0091 | -0.0263 | -0.0204 | 0.0145 | 0.0097 | 0.0080 | 0.0143 | 0.0105 |
| 1.4 | 0.0096 | 0.0086 | 0.0088 | -0.0226 | -0.0169 | 0.0125 | 0.0087 | 0.0072 | 0.0121 | 0.0086 |
| 1.6 | 0.0093 | 0.0084 | 0.0074 | -0.0200 | -0.0162 | 0.0111 | 0.0079 | 0.0065 | 0.0103 | 0.0072 |
| 1.8 | 0.0089 | 0.0077 | 0.0054 | -0.0187 | -0.0171 | 0.0101 | 0.0073 | 0.0059 | 0.0090 | 0.0066 |
| 2.0 | 0.0084 | 0.0064 | 0.0029 | -0.0185 | -0.0188 | 0.0092 | 0.0067 | 0.0056 | 0.0081 | 0.0064 |
| 2.5 | 0.0064 | 0.0021 | -0.0040 | -0.0203 | -0.0237 | 0.0078 | 0.0061 | 0.0057 | 0.0075 | 0.0079 |
| 3.0 | 0.0034 | -0.0028 | -0.0097 | -0.0231 | -0.0272 | 0.0071 | 0.0061 | 0.0065 | 0.0082 | 0.0097 |
| 3.5 | 0.0003 | -0.0068 | -0.0128 | -0.0254 | -0.0283 | 0.0068 | 0.0064 | 0.0068 | 0.0090 | 0.0099 |
| 4.0 | -0.0025 | -0.0095 | -0.0135 | -0.0265 | -0.0275 | 0.0067 | 0.0065 | 0.0064 | 0.0091 | 0.0080 |
| 4.5 | -0.0049 | -0.0109 | -0.0127 | -0.0264 | -0.0253 | 0.0066 | 0.0063 | 0.0053 | 0.0080 | 0.0045 |
| 5.0 | -0.0066 | -0.0112 | -0.0110 | -0.0255 | -0.0224 | 0.0064 | 0.0057 | 0.0038 | 0.0060 | 0.0000 |
| 5.5 | -0.0077 | -0.0108 | -0.0088 | -0.0240 | -0.0194 | 0.0061 | 0.0048 | 0.0022 | 0.0033 | -0.0047 |
| 6.0 | -0.0083 | -0.0099 | -0.0065 | -0.0222 | -0.0166 | 0.0057 | 0.0038 | 0.0008 | 0.0002 | -0.0093 |
| 6.5 | -0.0085 | -0.0086 | -0.0043 | -0.0203 | -0.0142 | 0.0052 | 0.0028 | -0.0004 | -0.0030 | -0.0135 |
| 7.0 | -0.0084 | -0.0072 | -0.0022 | -0.0185 | -0.0123 | 0.0046 | 0.0019 | -0.0013 | -0.0062 | -0.0173 |
| 7.5 | -0.0080 | -0.0058 | -0.0002 | -0.0168 | -0.0110 | 0.0040 | 0.0010 | -0.0020 | -0.0093 | -0.0207 |
| 8.0 | -0.0075 | -0.0043 | 0.0015 | -0.0154 | -0.0101 | 0.0034 | 0.0003 | -0.0023 | -0.0122 | -0.0236 |
| 8.5 | -0.0068 | -0.0029 | 0.0032 | -0.0142 | -0.0097 | 0.0029 | -0.0003 | -0.0025 | -0.0150 | -0.0263 |
| 9.0 | -0.0061 | -0.0015 | 0.0046 | -0.0133 | -0.0097 | 0.0023 | -0.0007 | -0.0024 | -0.0175 | -0.0286 |
| 9.5 | -0.0053 | -0.0001 | 0.0060 | -0.0126 | -0.0099 | 0.0018 | -0.0011 | -0.0023 | -0.0199 | -0.0306 |
| 10.0 | -0.0045 | 0.0011 | 0.0071 | -0.0121 | -0.0102 | 0.0014 | -0.0013 | -0.0020 | -0.0221 | -0.0323 |
| 12.0 | -0.0011 | 0.0053 | 0.0107 | -0.0116 | -0.0117 | 0.0003 | -0.0012 | -0.0004 | -0.0287 | -0.0362 |
| 14.0 | 0.0019 | 0.0083 | 0.0128 | -0.0117 | -0.0118 | -0.0002 | -0.0005 | 0.0011 | -0.0323 | -0.0363 |
| 16.0 | 0.0044 | 0.0105 | 0.0139 | -0.0114 | -0.0099 | -0.0001 | 0.0004 | 0.0022 | -0.0335 | -0.0337 |
| 18.0 | 0.0064 | 0.0118 | 0.0143 | -0.0103 | -0.0071 | 0.0002 | 0.0013 | 0.0030 | -0.0328 | -0.0297 |
| 20.0 | 0.0080 | 0.0126 | 0.0141 | -0.0087 | -0.0042 | 0.0006 | 0.0019 | 0.0034 | -0.0309 | -0.0252 |

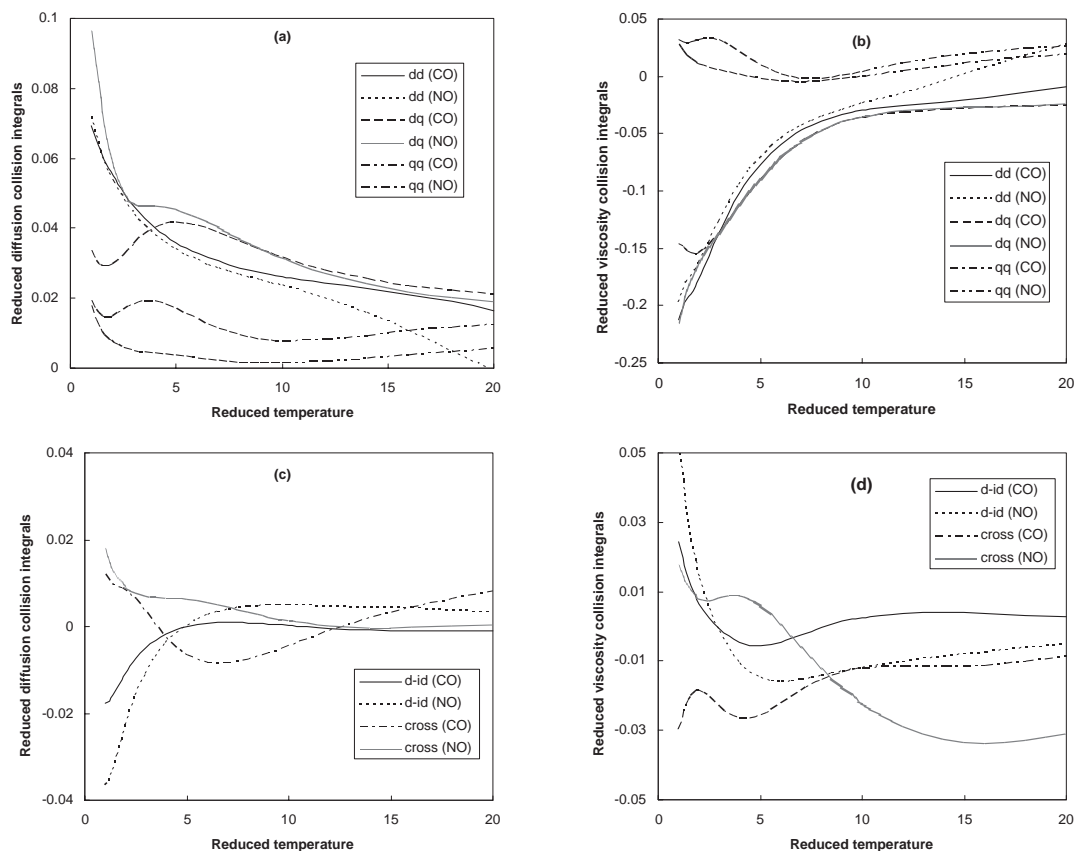


Fig. 1. Electrostatic and inductive contributions to the reduced collision integrals of CO and NO.

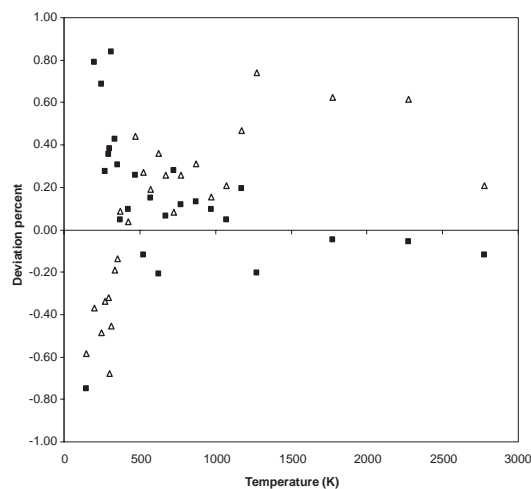


Fig. 2. Deviation percent between the calculated and experimental values²³ of the viscosity coefficients of NO (■) and CO (△).

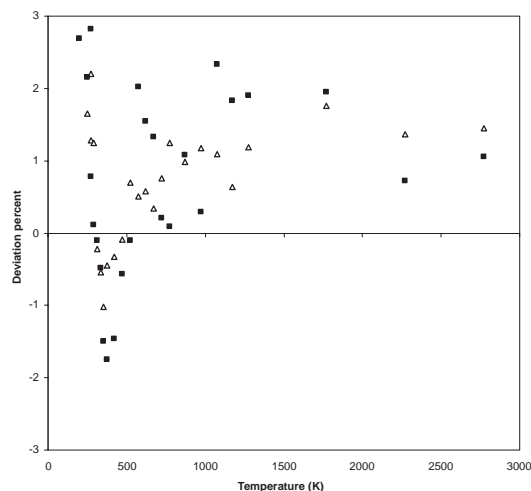


Fig. 3. Deviation percent between the calculated and experimental values²³ of the diffusion coefficients of NO (■) and CO (△).

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