Mutual Intersection Points of Reduced Collision Integrals for Lennard–Jones (n-m), Hulburt–Hirschfelder, and Tang–Toennies Potential Energy Functions

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Abstract
We investigate the reduced collision integrals \( \Omega^{(\ell, s)}(T^*) \) for \( 1 \leq \ell \leq 4 \), \( \ell \leq s \leq 7 \) and \( \ell + s \leq 8 \) for several isotropic potential energy functions: the Lennard–Jones \((n - m)\), the Hulburt–Hirschfelder, and Tang–Toennies potential. It is observed that for a given \( \ell \) and \( s \), \( \Omega^{(\ell, s)}(T^*) \) shows a mutual intersection region at a reduced temperature \( 0.39 < T^* = T^*_\ell s < 2.22 \) which is nearly independent of the potential energy function used.

Keywords Collision integrals · Intermolecular interaction potentials · Transport properties

1 Introduction
There is still a vivid interest in the transport properties of neat gases and gas mixtures. In particular, the calculation of transport properties such as diffusion and viscosity from binary potential energy functions \( U(r) \) becomes more and more relevant and also accurate, see, e.g., [1–11] and references therein. In many of these theoretical investigations, it is required to explicitly calculate the collision integrals [12, 13]. They occur in calculations of the transport coefficients. In the following, we neglect quantum effects. In terms of reduced units, the reduced collision integrals \( \Omega^{(\ell, s)}(T^*) \) are given by [12]

\[
\Omega^{(\ell, s)}(T^*) = \frac{2}{(s + 1)!T^*\ell^{2s+2}} \int_0^\infty e^{-g^*/T^*} g^{2s+3} Q^{(\ell, s)} d g^*,
\]

(1)
Reduced quantities are used throughout this formulation: \( T^* = kT/\varepsilon, \ r^* = r/\sigma, \ b^* = b/\sigma, \ U^* = U/\varepsilon, \) and \( g^* = \mu v^2 / 2\varepsilon. \) In addition, \( r^* \) is the largest real solution of the equation \( 1 - (b^*/r^*)^2 - U^*(r^*)/g^* = 0. \) \( b \) is the impact parameter, \( r \) the intermolecular distance, \( -\varepsilon \) the lowest energy of the potential energy function, \( U(\sigma) = 0, \mu \) and \( \nu \) are the reduced mass and the relative velocity of the colliding pair, respectively.

Despite of their simple structure as a threefold integral, it is known for a long time that the calculation of the reduced collision integrals is difficult. Therefore, a number of mathematical techniques and computer programs are available either for a classical or a full quantal treatment [4–6, 14–17]. In recent years, the reduced collision integrals have been calculated for several very accurate ab initio potential energy functions \( U(r). \) However, ab initio potentials are only available in the case of atoms and small molecules, see, e.g., [8–10, 18–20]. Due to the complexity of the problem, much simpler and therefore approximate potential energy functions \( U(r) \) are still widely in use [14]. For some of these potential energy models, extensive tables and fitting formulae of \( \Omega(\ell, s)(T^*) \) are given in the literature [2, 12, 14, 21–26].

Within the extended law of corresponding states, it has been observed that at least in the range \( 1 \lesssim T^* \lesssim 10 \Omega^{(1,1)*}(T^*) \) and \( \Omega^{(2,2)*}(T^*) \) are a function of \( T^* \) only irrespective of the underlying potential energy function [14, 25, 27–31]. This means despite of the different potentials \( U(r) \) for different atoms and molecules, \( \Omega^{(1,1)*}(T^*) \) in a limited temperature range is the same for all species considered. However, we have observed that the reduced collision integrals do not strictly follow the predicted corresponding states principle. Instead of showing a similar behavior in a limited range of approximately \( \Delta T^* \approx 9, \) there exists a very small single intersection region at a reduced temperature \( T^* \). For a given pair of \( \ell \) and \( s, \) this region to a very good extend is independent of the reduced intermolecular interaction potential \( U^* \) considered. In a very limited number of publications, this fact might have been observed by chance but lacks of any discussion [32]. In the present paper, a thorough detection and discussion of this intersection point are presented. Throughout this work, we only concentrate on isotropic potential energy functions of non-polar molecules since, in other cases, a different treatment of our problem seems to be in order [33, 34].

\[
Q^{(\ell)*}(g^*) = \frac{2}{1 - \frac{1}{2} \frac{1}{1 + \ell^*}} \int_0^\infty (1 - \cos \varphi) db^*, \tag{2}
\]

\[
\chi(b^*, g^*) = \pi - 2b^* \int_{r^*}^{\infty} \frac{dr^*}{r^*} \sqrt{1 - (b^*/r^*)^2 - U^*(r^*)/g^*}. \tag{3}
\]
2 Theory

The reduced collision integrals $\Omega^{(\ell,s)\ast}$ can be used to correct the transport properties of hard spheres for real gas behavior [12]. In the case of dilute gases which are considered throughout this work, this correction is shown below for the shear viscosity $\eta$

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

(4)

and self-diffusion coefficient $D$

$$D = \frac{3}{8 \rho} \frac{\sqrt{\pi m k T}}{\pi \sigma^2} \frac{f_D}{\Omega^{(1,1)\ast}}.$$  

(5)

$\rho$ is the density of the gas. $f_\eta$ and $f_D$ are higher-order correction factors

$$f_\eta = 1 + \frac{3}{196} (8E^\ast - 7)^2,$$

(6)

$$f_D = 1 + \frac{(6C^\ast - 5)^2}{8(2A^\ast + 5)},$$

(7)

which are also functions of the reduced collision integrals according to [12, 25]

$$A^\ast = \frac{\Omega^{(2,2)\ast}}{\Omega^{(1,1)\ast}},$$

(8)

$$C^\ast = \frac{\Omega^{(1,2)\ast}}{\Omega^{(1,1)\ast}},$$

(9)

$$E^\ast = \frac{\Omega^{(2,3)\ast}}{\Omega^{(2,2)\ast}}.$$  

(10)

It has been found that at moderate temperatures, $f_\eta$ and $f_D$ are in the order of unity [21, 23].

The reduced collision integrals are a function of the reduced temperature $T^\ast$. According to Eq. 1, they crucially depend on the intermolecular interaction potential $U^\ast$. In this study, three different models of $U^\ast(r^\ast)$ are taken into account.

The Lennard–Jones (n-m) potential

$$U^\ast_{LJ}(r^\ast) = \frac{m}{n - m} \frac{n}{n - n-m} \left( \left( \frac{1}{r^\ast} \right)^{n} - \left( \frac{1}{r^\ast} \right)^{m} \right),$$

(11)

the Hulburt–Hirschfelder potential

$$U^\ast_{HH}(r^\ast) = \exp[-2\alpha(r^\ast/d - 1)] - 2 \exp[-\alpha(r^\ast/d - 1)]$$

$$+ \beta (r^\ast/d - 1)^3 [1 + \gamma (r^\ast/d - 1)] \exp[-2\alpha(r^\ast/d - 1)],$$

(12)

and the Tang–Toennies potential [35].
Although obviously first introduced by Mie [36], $U^*_{LJ}(r^*)$ nowadays is known as the Lennard–Jones (n-m) potential [12, 14, 37]. It has two adjustable parameters $n$ and $m$. For physical reasons in most cases, $m = 6$ is chosen. It can considered to be only of moderate accuracy. However, it is still widely in use in all areas of chemistry and physics ranging from the analysis of transport properties to quantum-chemical calculations of large molecules [38–42]. The Hulburt–Hirschfelder potential $U^*_{HH}(r^*)$ has three parameters $\alpha$, $\beta$, and $\gamma$. It is used vividly for high temperature applications [2, 17]. The Tang–Toennies potential $U^*_{TT}(r^*)$ has only one parameter $b$ to adjust, the coefficients $C_{2n}^*$ being the reduced dispersion interaction energy constants. The Tang–Toennies potential was especially designed for the noble gases helium to radon and their binary mixtures [35].

$$U^*_{TT}(r^*) = \exp(-br^*) - \sum_{n=3}^{N} f_{2n}(br^*) C_{2n}^* r^{2n},$$

$$(13)$$

$$f_{2n}(x) = 1 - \exp(-x) \sum_{k=0}^{2n} \frac{x^k}{k!}.$$

3 Calculations

3.1 General Codes

In order to calculate the reduced collision integrals $\Omega^{(\epsilon,s)*}(T^*)$, two different program suites have been developed. First a Fortran program (F) has been written according to a procedure proposed by Colonna and Laricchiuta [15]. This program allows for a fast and reliable calculation of $\Omega^{(\epsilon,s)*}(T^*)$ over a broad temperature range. In our case, it was especially designed for the Lennard–Jones (n-m) potential. The evaluation time is about 1 s per data point on a standard laptop with an Intel i7 processor and 32 GB RAM memory. For this potential, we systematically calculate the reduced collision integrals $\Omega^{(\epsilon,s)*}(T^*)$ for $1 \leq \ell \leq 4$, $\ell \leq s \leq 7$ and $\ell + s \leq 8$ for $m = 6$ and $n = 12, 15, 20, 30$, and 50 as well as for the (n-m) pairs (9-6), (20-8), (20-9), and (28-7). We mainly concentrate on the range between $0.01 \leq T^* \leq 100.0$. In these ranges, our Fortran code allows for a robust screening with a relative accuracy of $\Delta\Omega^{(\epsilon,s)*}/\Omega^{(\epsilon,s)*} \leq 0.2 \%$ as can be seen by comparison to literature values and highly accurate calculations with Mathematica [43] as described below. The comparison is shown in Table 1. From the entries, it can be deduced that the results presented in the literature can be reproduced successfully.

Second, we use a straightforward Mathematica [43] code (M) for the calculation of the reduced collision integrals $\Omega^{(\epsilon,s)*}(T^*)$. We have made the observation that the default values of the Mathematica routines are able to handle automatically nearly all of the difficulties which occur during the course of the calculation of $\Omega^{(\epsilon,s)*}(T^*)$. The use of Mathematica routines has been described in the literature before [17, 44], but was hardly used up to now. Our code is given in the Appendix and is much simpler than the few other codes described in the
In order to check the quality of this code, we compare our findings for the Lennard–Jones (12-6) potential to the highly accurate calculations performed by Kim and Monroe [16] in Table 2. The latter authors state an accuracy of seven digits past the decimal compared to previously reported values at two reduced temperatures of $T^* = 0.3$ and 400.0. As can be seen, the Mathematica code is able to reproduce the results of Kim and Monroe [16] to a very good extend in the case of low and high temperatures. Our fast code F, however, fails at the highest reduced temperature $T^*$ of 400 and is therefore only recommended to be used up to $T^* = 100$. A severe drawback of code M is its quite long calculation time which severely depends on the parameters $U^*$ and $T^*$. It varies between 1 min (high temperature, LJ-potential) and about 60 min (low temperature, TT potential) per single point on a standard laptop with an Intel i7 processor and 32 GB RAM memory. We conclude from an inspection of Tables 1 and 2 that the routines used in this work yield trustworthy results of the reduced collision integrals. However, due to its superior accuracy, our Mathematica code was used for all single-point calculations for the Lennard–Jones (n-m), Tang–Toennies [35], and Hulburt–Hirschfelder potential [2, 17]. The Tang–Toennies potential is used

### Table 1: Reduced collision integrals $\Omega^{(\ell,s)}$ of the Lennard–Jones (m-n) potential calculated with Mathematica [43] (M) and Fortran (F) in comparison with the results given by Smith et al. [21]

| $(m,n)$ | $(\ell,s)$ | $T^*$ | Smith et al. (M), This work (F), This work compared to Ref. [21] | $10^4 \Delta \Omega/\Omega$, (M) compared to Ref. [21] | $10^4 \Delta \Omega/\Omega$, (F) compared to Ref. [21] |
|---------|------------|-------|-------------------------------------------------|------------------------|------------------------|
| (9,6)   | (1,1)      | 0.01  | 10.42147 10.42122 10.42275 − 0.24 1.23         | 0.015 9.09684 9.09390 9.06200 − 3.23 0.70         |
|         |            | 0.015 | 9.09684 9.09390 9.06200 − 3.23 0.70            | 9.73563 4.73161 4.73249 − 8.50 6.63         |
|         |            | 1.0   | 1.48479 1.48671 1.48687 12.93 14.01           | 1.48479 1.48671 1.48687 12.93 14.01         |
|         |            | 100.0 | 0.44668 0.44671 0.44689 0.67 4.70            | 0.44668 0.44671 0.44689 0.67 4.70         |
| (2,2)   | (1,1)      | 0.01  | 10.38493 10.37600 10.38037 − 8.60 4.39         | 9.05584 9.04680 9.05038 − 9.98 6.03         |
|         |            | 0.015 | 9.05584 9.04680 9.05038 − 9.98 6.03            | 4.72483 4.72955 4.73105 9.98 13.16         |
|         |            | 0.1   | 1.65766 1.65700 1.65731 − 3.98 2.11           | 1.65766 1.65700 1.65731 − 3.98 2.11         |
|         |            | 100.0 | 0.51772 0.51775 0.51840 0.58 13.13           | 0.51772 0.51775 0.51840 0.58 13.13         |
| (28,7)  | (1,1)      | 0.01  | 5.06535 5.06722 5.06881 3.69 6.83            | 4.51093 4.51290 4.51390 4.37 6.58         |
|         |            | 0.015 | 4.51093 4.51290 4.51390 4.37 6.58            | 2.63357 2.63450 2.63522 3.52 6.27         |
|         |            | 0.1   | 1.32097 1.32035 1.32048 − 4.69 3.71           | 1.32097 1.32035 1.32048 − 4.69 3.71         |
|         |            | 100.0 | 0.72373 0.72373 0.72392 0.00 2.63            | 0.72373 0.72373 0.72392 0.00 2.63         |
| (2,2)   | (1,1)      | 0.01  | 5.39494 5.40611 5.40865 20.70 25.41          | 5.39494 5.40611 5.40865 20.70 25.41         |
|         |            | 0.015 | 4.81089 4.82057 4.82264 20.12 24.42          | 2.82496 2.83144 2.83236 22.94 26.20         |
|         |            | 0.1   | 1.42971 1.43034 1.43064 4.41 6.50            | 1.42971 1.43034 1.43064 4.41 6.50         |
|         |            | 100.0 | 0.77185 0.77186 0.77233 0.13 6.21          | 0.77185 0.77186 0.77233 0.13 6.21         |
Table 2 Reduced collision integrals $\Omega^{(\varepsilon,s)}$ of the Lennard–Jones (12-6) potential calculated in this work with Mathematica [43] (M) and Fortran program (F) in comparison with highly accurate results given by Kim and Monroe [16] and early calculations of Hirschfelder et al. [12]

| $T^*$  | $(\varepsilon,s)$ | (M), This work | (F), This work | Kim and Monroe [16] | Hirschfelder et al. [12] | (M) $10^6 \Delta\Omega/\Omega$ comp. to [16] | (M) $10^2 \Delta\Omega/\Omega$ comp. to [12] | (F) $10^2 \Delta\Omega/\Omega$ comp. to [16] | (F) $10^2 \Delta\Omega/\Omega$ comp. to [12] |
|--------|------------------|----------------|----------------|---------------------|--------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| 0.3    | (1,1) 0.3489 675 | 2.6 505 535     | 2.6 500 024     | 2.662               | – 7.1                    | – 0.45                      | 0.02                        | – 0.43                      |
|        | (2,2) 1.9 664 634 | 2.2 571 778     | 2.2 568 342     | 2.256               | – 23.4                   | 0.03                        | 0.02                        | 0.25                        |
|        | (2,3) 2.8 436 584 | 2.8 446 945     | 2.8 436 719     | 2.785               | – 4.8                    | 2.11                        | 0.04                        | 2.14                        |
|        | (4,4) 2.8 436 584 | 2.5 806 076     | 2.5 806 610     | 2.535               | – 20.7                   | 1.80                        | 0.03                        | 1.83                        |
|        | (2,2) 2.5 806 076 | 2.5 806 076     | 2.5 806 610     | 2.535               | – 20.7                   | 1.80                        | 0.03                        | 1.83                        |
|        | (2,3) 2.3 622 351 | 2.3 629 479     | 2.3 622 719     | 2.333               | – 15.6                   | 1.25                        | 0.03                        | 1.28                        |
|        | (2,4) 2.1 704 110 | 2.1 708 851     | 2.1 704 207     | 2.152               | – 4.5                    | 0.86                        | 0.02                        | 0.88                        |
|        | (2,6) 2.0 010 611 | 2.0 014 232     | 2.0 010 465     | 1.990               | 7.3                      | 0.56                        | 0.02                        | 0.57                        |
|        | (4,4) 2.5 710 030 | 2.5 719 354     | 2.5 710 549     | 2.557               | – 20.1                   | 0.55                        | 0.03                        | 0.58                        |
| 400.0  | (1,1) 0.4 141 855 | 0.3 597 421     | 0.4 418 524     | 0.4170              | – 0.67                   | 0.68                        | – 13.14                     | – 13.73                     |
|        | (1,2) 0.3 918 901 | 0.2 818 961     | 0.3 188 997     | 0.3955              | 0.34                     | – 0.91                      | – 28.07                     | – 28.72                     |
|        | (1,3) 0.3 759 885 | 0.2 016 892     | 0.3 598 843     | 0.3802              | 0.18                     | – 1.11                      | – 46.36                     | – 46.95                     |
|        | (2,2) 0.4 710 329 | 0.4 597 367     | 0.4 103 246     | 0.4811              | 0.82                     | – 2.09                      | – 2.40                      | – 4.44                      |
|        | (2,3) 0.4 522 682 | 0.4 234 396     | 0.4 226 789     | 0.4638              | 0.76                     | – 2.49                      | – 6.37                      | – 8.70                      |
|        | (2,4) 0.4 377 739 | 0.3 793 480     | 0.4 377 361     | 0.4502              | 0.73                     | – 2.76                      | – 13.34                     | – 15.74                     |
|        | (2,5) 0.4 260 365 | 0.3 258 880     | 0.4 203 617     | 0.4393              | 0.67                     | – 3.02                      | – 23.51                     | – 25.82                     |
|        | (2,6) 0.4 162 166 | 0.2 657 647     | 0.4 121 633     | 0.4302              | 0.62                     | – 3.25                      | – 36.15                     | – 38.22                     |
|        | (4,4) 0.4 588 874 | 0.4 470 537     | 0.4 888 704     | 0.4758              | 0.78                     | – 3.55                      | – 2.58                      | – 6.04                      |
for all neat noble gases from helium to radon. The Hulburt–Hirschfelder potential has been applied to argon and the (H⁺·He)-pair. All potential parameters can be found in the corresponding literature [2, 17, 35].

4 Results and Discussion

We have used a very simple detection scheme for the mutual intersection points of the reduced collision integrals. First of all, we have used the Lennard–Jones (n-6) potential with n = 12, 15, 20, 30, and 50 and have calculated all the reduced collision integrals Ω_LJ^{(\ell,s)\epsilon}(T^*) in the range 1.0 ≤ T^* ≤ 5.0. The index LJ denotes that the reduced collision integrals are calculated for the Lennard–Jones (n-m) potential. A typical plot is shown in Fig. 1. The resulting curves show a systematic dependence on the parameter n. The most suitable reduced intersection temperature $T^*_{\ell,s}$ is extracted by visual inspection. At worst all intersections are safely lying inside an interval of $\Delta T^*_{\ell,s} = 0.1$, where this maximum range is observed for the $\ell = 1$ and $s = 1$ pair. A typical example of this determination is shown in Fig. 1. All values of $T^*_{\ell,s}$ are given in Table 3. After $T^*_{\ell,s}$ was fixed, we calculate in addition $Ω_LJ^{(\ell,s)\epsilon}(T^*)$ for the Lennard–Jones (n-6) potentials with n = 9, 100, 400, 500, 600, and 700. The mean $Ω_LJ^{(\ell,s)\epsilon}(T^*)$ over all 11 different values of n is displayed in Table 3. Subsequently, $Ω_{TT}^{(\ell,s)\epsilon}(T^*)$ was calculated for the Tang–Toennies (TT) and Hulburt–Hirschfelder (HH) potentials. The results $Ω_{TT}^{(\ell,s)\epsilon}(T^*)$ and $Ω_{HH}^{(\ell,s)\epsilon}(T^*)$ are also given in Table 3.

Overall, the reduced intersection temperatures $T^*_{\ell,s}$ are found in the range 0.39 < $T^*_{\ell,s}$ < 2.22. For typical values of $(\epsilon/k)$, this range indicates moderate temperatures $T$ and is not located at extremely high or low temperatures. For a given value of

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![Fig. 1](image)  
**Fig. 1** Visual determination of the approximate intersection point as exemplified for the reduced collision integral $Ω_LJ^{(2,2)\epsilon}(T^*)$. The dotted rectangle shows the range where the individual intersections for the Lennard–Jones (n-6) potential are found. The dimension of this range is given by $\Delta T^* = 0.012$ and $\Delta Ω^{(2,2)\epsilon} = 0.002$
Table 3  Observed values of $T_{\ell,s}^*$ for which $\Omega_{\text{LJ}}^{(\varepsilon,s)^*}(T_{\ell,s}^*)$ calculated for the Lennard–Jones (n-6) potential is virtually independent of $9 \leq n \leq 700$, see also Fig. 2.

| $(\varepsilon,s)$ | $T_{\ell,s}^*$ | $\Omega_{\text{LJ}}^{(\varepsilon,s)^*}(T_{\ell,s}^*)$ | $\Omega_{\text{TT}}^{(\varepsilon,s)^*}(T_{\ell,s}^*)$ | $\Omega_{\text{HH}}^{(\varepsilon,s)^*}(T_{\ell,s}^*)$ |
|-----------------|----------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| (1,1)           | 1.610          | 1.1487                                        | 1.1458                                        | 1.1426                                        | 1.1428                                        |
| (1,2)           | 1.066          | 1.1590                                        | 1.1568                                        | 1.1538                                        | 1.1543                                        |
| (1,3)           | 0.794          | 1.1639                                        | 1.1621                                        | 1.1622                                        | 1.1592                                        | 1.1600                                        |
| (1,4)           | 0.630          | 1.1678                                        | 1.1663                                        | 1.1664                                        | 1.1635                                        | 1.1645                                        |
| (1,5)           | 0.523          | 1.1691                                        | 1.1678                                        | 1.1680                                        | 1.1650                                        | 1.1663                                        |
| (1,6)           | 0.450          | 1.1665                                        | 1.1654                                        | 1.1656                                        | 1.1626                                        | 1.1643                                        |
| (1,7)           | 0.394          | 1.1654                                        | 1.1645                                        | 1.1646                                        | 1.1619                                        | 1.1635                                        |
| (1,8)           | 2.213          | 1.1292                                        | 1.1282                                        | 1.1283                                        | 1.1261                                        | 1.1270                                        |
| (2,1)           | 1.645          | 1.1326                                        | 1.1317                                        | 1.1319                                        | 1.1297                                        | 1.1307                                        |
| (2,2)           | 1.317          | 1.1316                                        | 1.1309                                        | 1.1311                                        | 1.1289                                        | 1.1301                                        |
| (2,3)           | 1.087          | 1.1343                                        | 1.1339                                        | 1.1337                                        | 1.1338                                        | 1.1328                                        |
| (2,4)           | 0.930          | 1.1343                                        | 1.1339                                        | 1.1337                                        | 1.1338                                        | 1.1328                                        |
| (3,1)           | 1.344          | 1.1474                                        | 1.1456                                        | 1.1457                                        | 1.1431                                        | 1.1437                                        |
| (3,2)           | 1.075          | 1.1483                                        | 1.1474                                        | 1.1467                                        | 1.1468                                        | 1.1449                                        |
| (3,3)           | 0.891          | 1.1508                                        | 1.1499                                        | 1.1493                                        | 1.1495                                        | 1.1468                                        |
| (4,4)           | 1.679          | 1.1237                                        | 1.1233                                        | 1.1230                                        | 1.1231                                        | 1.1220                                        | 1.1221                                        | 1.1221                                        | 1.1191                                        |

The mean $\Omega_{\text{LJ}}^{(\varepsilon,s)^*}(T_{\ell,s}^*)$ as well as the corresponding values $\Omega_{\text{TT}}^{(\varepsilon,s)^*}(T_{\ell,s}^*)$ and $\Omega_{\text{HH}}^{(\varepsilon,s)^*}(T_{\ell,s}^*)$ for the Tang–Toennies (TT) and Hulburt–Hirschfelder (HH) potentials, respectively, are given in columns 3–11. All entries are calculated with Mathematica code. The results are partly displayed in Figs. 3, 4, 5, 6, 7 and 8.
ℓ \ T^*_s \), decreases monotonically with increasing \( s \), see Table 3. The individual results \( \Omega^{(ℓ,s)}_{LJ}(T^*_s) \) for each \( n \) are shown in full detail in Fig. 2. The largest scattering can be seen in the case of the \((ℓ, s) = (1, 1)\) pair. In all other cases, only a moderate dependence of \( \Omega^{(ℓ,s)}_{LJ}(T^*_s) \) on \( n \) is observed. Therefore, an arithmetic mean \( \bar{\Omega}^{(ℓ,s)}_{LJ}(T^*_s) \) of all \( n \) is calculated for a given \((ℓ, s)\) pair. As can be seen from Table 3, \( \Omega^{(ℓ,s)}_{LJ}(T^*_s) \) varies only slightly between 1.12 < \( \Omega^{(ℓ,s)}_{LJ}(T^*_s) < 1.18 \). The individual results of \( \Omega^{(ℓ,s)}_{LJ}(T^*_s) \) for different \( n \) in Fig. 2 are clustered in groups for \( ℓ = 1, ℓ = 3, ℓ = 2, \) and \( ℓ = 4 \) (from top to bottom). On account of this observation, an averaging over \( s \) for a given value of \( ℓ \) is carried out according to Eq. (14). The result is also shown in Fig. 2.

\[
\bar{\Omega}^{(ℓ,s)} = \frac{1}{9 - 2\ell} \sum_{s=\ell}^{8-\ell} \Omega^{(ℓ,s)}_{LJ}(T^*_s), \quad (14)
\]

We now compare our findings for all three potentials, see Eqs. 11–13. For some pairs, \((ℓ, s)\) the calculated reduced collision integrals \( \Omega^{(ℓ,s)}(T^*) \) are shown in Figs. 3, 4, 5, 6, 7, and 8. In these figures, we have also included results for the Lennard–Jones (20-8) and (20-9) potential. In all cases, the curves seem to intersect in one point. This supports our findings concerning the mutual intersection point of the reduced collision integrals for a limited class of isotropic potential energy functions. Numerical results of \( \Omega^{(ℓ,s)}_{TT}(T^*_s) \) and \( \Omega^{(ℓ,s)}_{HH}(T^*_s) \) for all pairs of \( ℓ \) and \( s \) are given in Table 3. First, it can be seen in full detail that in all cases, \( \Omega^{(ℓ,s)}_{LJ}(T^*_s) \approx \Omega^{(ℓ,s)}_{TT}(T^*_s) \approx \Omega^{(ℓ,s)}_{HH}(T^*_s) \). This is also outlined in Figs. 3, 4, 5, 6, 7, and 8. A closer look reveals that in general \( \Omega^{(ℓ,s)}_{TT}(T^*_s) \) is lower than \( \Omega^{(ℓ,s)}_{HH}(T^*_s) \). The largest relative deviation of \( \approx 2 \% \) is observed for the \((ℓ, s) = (1, 1)\) pair. For a given \((ℓ, s)\) pair, \( \Omega^{(ℓ,s)}_{TT}(T^*_s) \) only shows a small relative variation of not more than 0.5 \% across the results for all 6 noble gases.

The results for the Hulbert–Hirschfelder potential show a somewhat more pronounced behavior. \( \Omega^{(ℓ,s)}_{TT}(T^*_s) \) for argon agrees very well with \( \Omega^{(ℓ,s)}_{LJ}(T^*_s) \) of the Lennard–Jones potential. The only exception again is found for \((ℓ, s) = (1, 1)\) where a relative deviation of 0.7 \% is observed. In the case of the H⋅⋅He pair, the disagreement is generally higher and a maximum relative deviation for \((1,1)\) of 2.5 \% is detected.

It can be stated that for the three different potential energy models investigated here, a mutual intersection point or at least a tiny mutual intersection region around \( \Omega^{(ℓ,s)}(T^*_s) \) for a given pair of \( ℓ \) and \( s \) exists. This mutual intersection region has not been described in the literature before and, therefore, is remarkable by itself.

From this observation, a simple conclusion can be drawn. We consider the transport coefficients viscosity \( \eta \) and self-diffusion \( D \) which are already given in Eqs. 4 and 5. In the latter case, we now consider the coefficient \( \rho D \). To a first approximation, we set the small correction factors \( f_\eta \approx f_D \approx 1 \). We define the ratio \( R(α, T) \) with \( α > 0 \) via

\[
R(α, T) = \frac{\eta(αT)}{\rho D(T)} = \frac{5}{16} \frac{\sqrt{πmkT}}{α^2} \frac{1}{\Omega^{(2,2)*}(αT^*)} = \frac{5}{6} \frac{\sqrt{πmkT}}{8} \frac{1}{\Omega^{(1,1)*}(T^*)} \frac{1}{\Omega^{(2,2)*}(αT^*)}. \quad (15)
\]
In principle, the left-hand side can be determined from experiment. In order to proceed, we recall that the intersection points of the reduced collision integrals obtained from the Lennard–Jones potential are given by
\[ \Omega(2,2) \approx 2.213 \] and
\[ \Omega(1,1) \approx 1.61. \] These points are
\[ \begin{align*}
\Omega(2,2) &= 2.213, \\
\Omega(1,1) &= 1.61.
\end{align*} \]

### Table 4

| Gas   | \( (\epsilon/k) = (T_0/1.61) \) | \( 10^{10} \sigma/k \) | \( 10^{10} \sigma/m \), from literature |
|-------|---------------------------------|-------------------------|----------------------------------------|
| Neon  | –                               | 32.8 [40], 42.3 [35]    | 2.820 [40], 2.768 [35]                 |
| Argon | 144.1                           | 93.3 [40], 155.0 [47], 143.4 [35] | 3.542 [40], 3.276 [47], 3.369 [35] |
| Krypton | 214.9                         | 178.9 [40], 221.0 [47], 201.5 [35] | 3.655 [40], 3.520 [47], 3.593 [35] |
| Xenon | 299.4                           | 231.0 [40], 310.9 [47], 282.9 [35] | 4.047 [40], 3.845 [47], 3.910 [35] |
| F₂    | 129.2                           | 112.6 [40], 136.9 [48]  | 3.357 [40], 3.298 [48]                 |
| Cl₂   | 460.9                           | 316.0 [40], 497.0 [48]  | 4.217 [40], 3.960 [48]                 |
| BF₃   | 226.1                           | 186.3 [40], 310.5 [49]  | 4.198 [40], 3.877 [49]                 |
| CH₄   | 221.1                           | 148.6 [40], 220.8 [47]  | 3.758 [40], 3.563 [47]                 |
| CF₄   | 272.0                           | 134.0 [40], 328.4 [49]  | 4.662 [40], 4.132 [47]                 |
| SF₆   | 121.7                           | 222.1 [40], 417.8 [49]  | 5.128 [40], 4.742 [47]                 |
| C₃H₈  | 370.2                           | 237.1 [40], 478.4 [50]  | 5.118 [40], 4.566 [50]                 |

**Fig. 3** Reduced collision integrals \( \Omega^{(1,1)} \) calculated with the Lennard–Jones (n-m), Eq. 11, Hulbert–Hirschfelder (HH), Eq. 12, and Tang–Toennies (TT), Eq. 13, potential. The parameters of the HH potential are taken from Buchowiecki [17] (Ar) and Bruno et al. [2] (H⁺He), the TT parameters are given by Tang and Toennies [35].

In principle, the left-hand side can be determined from experiment. In order to proceed, we recall that the intersection points of the reduced collision integrals obtained from the Lennard–Jones potential are given by
\[ \Omega^{(2,2)}(T_{22}^*) = 2.213 \] and
\[ \Omega^{(1,1)}(T_{11}^*) = 1.61. \] These points are...
Fig. 4 Reduced collision integrals $\Omega^{(1,2)*}$ calculated with the Lennard–Jones (n-m), Eq. 11, Hulburt–Hirschfelder (HH), Eq. 12, and Tang–Toennies (TT), Eq. 13, potential. The parameters of the HH potential are taken from Buchowiecki [17] (Ar) and Bruno et al. [2] (H$^+\cdot$He), the TT parameters are given by Tang and Toennies [35].

Fig. 5 Reduced collision integrals $\Omega^{(2,2)*}$ calculated with the Lennard–Jones (n-m), Eq. 11, Hulburt–Hirschfelder (HH), Eq. 12, and Tang–Toennies (TT), Eq. 13, potential. The parameters of the HH potential are taken from Buchowiecki [17] (Ar) and Bruno et al. [2] (H$^+\cdot$He), the TT parameters are given by Tang and Toennies [35].
Fig. 6 Reduced collision integrals $\Omega^{(2,3)*}$ calculated with the Lennard–Jones (n-m), Eq. 11, Hulburt–Hirschfelder (HH), Eq. 12, and Tang–Toennies (TT), Eq. 13, potential. The parameters of the HH potential are taken from Buchowiecki [17] (Ar) and Bruno et al. [2] (H–He), the TT parameters are given by Tang and Toennies [35].

Fig. 7 Reduced collision integrals $\Omega^{(3,3)*}$ calculated with the Lennard–Jones (n-m), Eq. 11, Hulburt–Hirschfelder (HH), Eq. 12, and Tang–Toennies (TT), Eq. 13, potential. The parameters of the HH potential are taken from Buchowiecki [17] (Ar) and Bruno et al. [2] (H–He), the TT parameters are given by Tang and Toennies [35].
nearly independent of the potential energy function considered. We now choose \( a = T_{11}^*/T_{22}^* = 1.375 \) and according to Eq. 15 obtain the ratio

\[
R(1.375, T) = \frac{5}{6} \sqrt{\frac{1.375}{\Omega^{(1,1)*}(T^*)}}. \tag{16}
\]

It is interesting to note that at \( T = T_0 = T_{11}^* (\epsilon/k) = T_{22}^* (\epsilon/k)/1.375 \), the ratio \( R(1.375, T_0) = 1.0036 \approx 1 \) is independent of the underlying potential energy function. Therefore, solving \( R(1.375, T_0) = 1.0036 \) for \( T_0 \) might give the possibility to determine the potential parameter \( (\epsilon/k) \) according to \( (\epsilon/k) = T_0/T_{11}^* = T_0/1.61 \). A plot of \( R(1.375, T) \) for \( \text{BF}_3, \text{F}_2, \text{Cl}_2, \text{CH}_4, \text{CF}_4, \text{SF}_6, \text{C}_3\text{H}_8 \), and the noble gases from neon to xenon is shown in Fig. 9. The intersection points with \( R(1.371, T_0) = 1.0036 \) are given in Table 4. It can be seen that in most cases, a good approximate value \( (\epsilon/k) \) of the potential well depth can be extracted from the plots. A severe outlier is observed for \( \text{SF}_6 \) whereas in the case of neon, this analysis fails completely.
The extraction of $\sigma$ is straightforward. Solving the numerators in Eq. 15 for $\sigma$, we obtain

$$\sigma = \left( \frac{5}{16} \sqrt{\frac{\pi mkaT}{\eta(\alpha T)}} \frac{1}{\Omega^{(2,2)*}(\alpha T^*)} \right)^{1/2}. \quad (17)$$

At $T = T_0$ and $\alpha = 1.375 = T_{22}^*/T_{11}^*$ $\sigma$ obtained from Eq. 17 does not depend on the potential energy function used in modeling the intermolecular interactions. With an experimental value of $\eta(1.375T_0)$ in Eq. 17, an estimate of $\sigma$ can be calculated. Results are also listed in Table 4. Again, we failed to obtain a result for neon. SF$_6$ seems to be a severe outlier. In all other cases fair agreement can be seen between the results presented in this work and data from the literature. It should be stressed that our procedure for obtaining $(\varepsilon/k)$ and $\sigma$ does not rely on the assumption of a specific potential energy model. It is therefore in principle superior to schemes which are explicitly using, e.g., the Lennard–Jones (12-6) potential for obtaining $(\varepsilon/k)$ and $\sigma$ [12, 16, 40]. However, it is severely hampered by the fact that both the viscosity and self-diffusion coefficient must be available over large temperature ranges with high accuracy. Although this might be possible for $\eta$ [45] at present, this is not feasible in the case of $\varrho D$ [46].

5 Conclusion

We have studied the reduced collision integrals $\Omega^{(\ell,s)*}(T^*)$ for the Lennard–Jones (n-m), Tang–Toennies, and Hulburt–Hirschfelder potential energy functions. We have detected a small intersection region with $\Delta T^* \leq 0.1$ of the reduced collision integrals $\Omega^{(\ell,s)*}(T^*)$, which for given $\ell$ and $s$ to a very good extent is independent of the underlying isotropic potential energy model. This conclusion was derived from a much more systematic and detailed look at the behavior of $\Omega^{(\ell,s)*}(T^*)$ compared to former studies presented in the literature. Indeed, in contrast to our findings, those studies have revealed an extended range of at least $\Delta T^* \approx 9$ where the reduced collision integrals can be described by a single analytical function irrespective of the potential energy function. Our studies so far have concentrated on isotropic potentials of atoms and non-polar molecules. For this class in principle, the potential parameters $\varepsilon$ and $\sigma$ can be extracted from measurements of $\eta$ and $D$ without the assumption of a specific potential energy model. It would be interesting to see in future works how $\Omega^{(\ell,s)*}(T^*)$ of polar molecules interacting via a Stockmayer potential energy function behave. To this end, it should be checked if the straightforward Mathematica code presented here is also able to handle the necessary integrations.
Appendix 1: Mathematica Notebook

Below, the general scheme of the Mathematica notebook used is displayed. In this example, the calculations are carried out for the Lennard–Jones (n-m) potential energy function Eq. 11, line In[13].

In[12] := NeuL[l_] := If[EvenQ[l], 2.0 + 2.0/l, 2.0]

In[13] := Ured[n_?NumericQ, m_?NumericQ, rred_] := m^(m/(m-n)) * n^(n/(n-m)) *(rred^(-n) - rred^(-m))/(n-m)

In[14] := ChiHilf[bred_, gred_, rred_, n_, m_] := 1.0 - rred^(-2.0)*bred^2.0 - Ured[n, m, rred]*gred^(-2.0)

In[15] := Testx[bred_?NumericQ, gred_?NumericQ, n_?NumericQ, m_?NumericQ] :=
Max[rred/.FindRoot[{ChiHilf[bred, gred, n, m]==0.0}, {rred, #},
AccuracyGoal->25, PrecisionGoal->25, WorkingPrecision->40, Method->
"Newton"][[1]]&/@{1.0,bred}

In[16] := Testn[bred_?NumericQ, gred_?NumericQ, n_?NumericQ, m_?NumericQ] :=
Min[rred/.FindRoot[{ChiHilf[bred, gred, n, m]==0.0}, {rred, #},
AccuracyGoal->25, PrecisionGoal->25, WorkingPrecision->40, Method->
"Newton"][[1]]&/@{1.0,bred}

In[17] := Nullstelle[bred_?NumericQ, gred_?NumericQ, n_?NumericQ, m_?NumericQ] :=
If[Abs[ChiHilf[bred, gred, Testx[bred, gred, n, m], n, m]]<10^-6,
Testx[bred, gred, n, m], Testn[bred, gred, n, m]]

In[18] := chi[gred_?NumericQ, bred_?NumericQ, n_, m_] :=
Pi - 2.0*bred*(NIntegrate[rred^(-2.0)*ChiHilf[bred, gred, rred, n, m]^(-0.5),
{rred, Nullstelle[bred, gred, n, m], Infinity}, Method->
{Automatic, "SymbolicProcessing"->0})

In[19] := Qlred[1_?NumericQ, gred_?NumericQ, n_?NumericQ, m_?NumericQ] :=
NeuL[1]*NIntegrate[(1.0-Cos[chi[gred, bred, n, m]]^"1")*bred,
{bred, 0.0, Infinity}, Method->{Automatic, "SymbolicProcessing"->0}]

In[20] := OmegaFullInt1min[1_, s_, gredmin_, Tred_, n_, m_,] :=
2.0*Tred^(-s-2.0)/((s+1)!)*NIntegrate[Qlred[1, gred, n, m]*
Exp[-gred^2.0*Tred]*gred^(-2.0*s+3.0),
{gred, gredmin, Infinity}, Method->{Automatic, "SymbolicProcessing"->0}]

Some difficulties have been observed.

1. In the case of the Tang–Toennies potential some of the reduced collision integrals are complex numbers \(\Omega^{(s)}(T^*) = A + Bi\). However, the ratio \(B/A\) is very small and in the range of \(10^{-7} \leq B/A \leq 10^{-5}\). By increasing the WorkingPrecision, AccuracyGoal, and PrecisionGoal, the imaginary part \(B\) in most cases can be forced to be \(B = 0\) without any noticeable change of the calculated \(A\)-value.
Therefore, we always take $\Omega^{(\varepsilon,s)}(T^*) = A$ even in cases where a complex number has been calculated.

2. In the case of the Lennard–Jones (n-m) potential with $n = 9$ the numerical calculation of $\Omega^{(\varepsilon,s)}(T^*)$ does not converge. In these cases it is advisable to set the lower integration bound $\text{gredmin}$ in In[20] to $\text{gredmin} = 0.002$. The error is very small and below 0.01 %, as can be seen in the case of $\Omega^{(1,1)}(T^* = 1.61)$. With $\text{gredmin} = 0.0$ the calculated value is 1.1623165, with $\text{gredmin} = 0.002$ a value of 1.1623253 results.

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References

1. E. Levi, J.R. Stallcop, H. Partridge, Transport properties of boron and aluminum. Theor. Chem. Acc. 103, 518–523 (2000)
2. D. Bruno, C. Catalfamo, M. Capitelli, G. Colonna, O. De Pascale, P. Diomede, C. Gorse, A. Laricchiusa, S. Longo, D. Giordano, F. Pirani, Transport properties of high-temperature Jupiter atmosphere components. Phys. Plasmas 17, 112315 (2010)
3. A.W. Jasper, E. Kamarchik, J.A. Miller, S.J. Klippenstein, First-principles binary diffusion coefficients for H, H₂, and four normal alkanes + N₂. J. Chem. Phys. 141, 124313 (2014)
4. F. Sharipov, V.J. Benites, Transport coefficients of helium–argon mixture based on ab initio potential. J. Chem. Phys. 143, 154104 (2015)
5. F. Sharipov, V.J. Benites, Transport coefficients of multi-component mixtures of noble gases based on ab initio potentials: viscosity and thermal conductivity. Phys. Fluids 32, 077104 (2020)
6. F. Sharipov, V.J. Benites, Transport coefficients of multicomponent mixtures of noble gases based on ab initio potentials: diffusion coefficients and thermal diffusion factors. Phys. Fluids 32, 097110 (2020)
7. F. Sharipov, V.J. Benites, Transport coefficients of isotopic mixtures of noble gases based on ab initio potentials. Phys. Chem. Chem. Phys. 23, 16664–16674 (2021)
8. B. Jäger, R. Hellmann, E. Bich, E. Vogel, State-of-the-art ab initio potential energy curve for the krypton atom pair and thermophysical properties of dilute krypton gas. J. Chem. Phys. 144, 114304 (2016)
9. R. Hellmann, Cross second virial coefficients and dilute gas transport properties of the systems (H₂S + C₃H₈), (C₂H₆ + C₃H₈), and (H₂S + C₃H₈) from ab initio-based intermolecular potentials. J. Chem. Eng. Data 65, 4712–4724 (2020)
10. R. Hellmann, C. Gaiser, B. Fellmuth, T. Vasyltsova, E. Bich, Thermophysical properties of low-density neon gas from highly accurate first-principles calculations and dielectric-constant gas thermometry measurements. J. Chem. Phys. 154, 164304 (2021)
11. R. Hellmann, A.H. Harvey, First-principles diffusivity ratios for atmospheric isotope fractionation on Mars and Titan. J. Geophys. Res. Planets 126, 2021 (2021)
12. J.O. Hirschfelder, C.F. Curtiss, R.B. Bird, Molecular Theory of Gases and Liquids (Wiley, New York, 1954)
13. S. Chapman, T.G. Cowling, The Mathematical Theory of Non-Uniform Gases (Cambridge University Press, Cambridge, 1970)
14. G.C. Maitland, M. Rigby, E.B. Smith, W.A. Wakeham, Intermolecular Forces (Oxford University Press, Oxford, 1981)
15. G. Colonna, A. Laricchiuta, General numerical algorithm for classical collision integral calculation. Comput. Phys. Commun. 178, 809–816 (2008)
16. S.U. Kim, C.W. Monroe, High-accuracy calculations of sixteen collision integrals for Lennard–Jones (12-6) gases and their interpolation to parameterize neon, argon, and krypton. J. Comput. Phys. 273, 358–373 (2014)
17. M. Buchowiecki, High-temperature collision integrals for m-6-8 and Hulburt–Hirschfelder potentials. Int. J. Thermophys. 43, 38 (2022)
18. K. Patkowski, K. Szalewicz, Argon pair potential at basis set and excitation limits. J. Chem. Phys. 133, 094304 (2010)
19. Y.N. Kalugina, A. Faure, A. van der Avoird, K. Walker, F. Lique, Interaction of H₂O with CO: potential energy surface, bound states and scattering calculations. Phys. Chem. Chem. Phys. 20, 5469–5477 (2018)
20. R. Hellmann, Cross second virial coefficient of the H₂O-CO system from a new ab initio pair potential. Int. J. Thermophys. 43, 25 (2022)
21. F.J. Smith, E.A. Mason, R.J. Munn, Transport collision integrals for gases obeying 9-6 and 28-7 potentials. J. Chem. Phys. 42, 1334–1339 (1965)
22. M. Klein, F.J. Smith, Tables of collision integrals for the (m,6) potential function for 10 values of m. J. Res. Natl. Bur. Stand. A Phys. Chem. 72A, 359–423 (1968)
23. S.T. Lin, H.W. Hsu, Transport collision integrals for gases using the Lennard–Jones (6, n) potentials. J. Chem. Eng. Data 14, 328–332 (1969)
24. P.D. Neufeld, A.R. Janzen, R.A. Aziz, Empirical equations to calculate 16 of the transport collision integrals Ω(\ell,s)\ast for the Lennard–Jones (12-6) potential. J. Chem. Phys. 57, 1100–1102 (1972)
25. J. Millat, J.H. Dymond, N. de Castro (eds.), Transport Properties of Fluids, Their Correlation, Prediction and Estimation (Cambridge University Press, Cambridge, 1996)
26. I. Coroiu, D.D. Demco, Second virial coefficients and transport properties of hexafluoride gases from an improved intermolecular potential. Z. Nat. 52a, 748–756 (1997)
27. J. Kestin, S.T. Ro, W. Wakeham, An extended law of corresponding states for the equilibrium and transport properties of the noble gases. Physica 58, 165–211 (1972)
28. B. Najafi, E.A. Mason, J. Kestin, Improved corresponding states principle for the noble gases. Physica 119, 387 (1983)
29. J. Bzowski, J. Kestin, E.A. Mason, F.J. Uribe, Equilibrium and transport properties of gas mixtures at low density: eleven polyatomic gases and five noble gases. J. Phys. Chem. Ref. Data 19, 1179–1232 (1990)
30. B. Najafi, Y. Ghayeb, G.A. Parsafar, New correlation functions for viscosity calculation of gases over wide temperature and pressure ranges. Int. J. Thermophys. 21, 1011–1031 (2000)
31. B. Haghighi, A.H. Djavanmardi, M. Najafi, Prediction of the transport properties of SF₆ with O₂, CO₂, CF₄, N₂ and CH₄ mixtures at low density by the inversion method (part II). J. Theor. Comput. Chem. 3, 69–90 (2004)
32. P.A. Vicharelli, Analytic parametrization of transport coefficients of Lennard–Jones (n,6) fluids. J. Appl. Phys. 62, 2250–2255 (1987)
33. M. Abbaspour, Transport, thermodynamic, and structural properties of fluid ammonia using a new intermolecular potential: the inversion method and molecular dynamics simulation. Chem. Phys. 389, 121–127 (2011)
34. M. Abbaspour, H. Akbarzadeh, S. Salemi, K. Pirfalak, Molecular dynamics simulation of liquid water and ice nanoclusters using a new effective HFD-like model. J. Comput. Chem. 39, 269–278 (2018)
35. K.T. Tang, J.P. Toennies, The van der Waals potentials between all the rare gas atoms from He to Rn. J. Chem. Phys. 118, 4976–4983 (2003)
36. G. Mie, Zur kinetischen Theorie der einatomigen Körper. Ann. Phys. 11, 657–697 (1903)
37. J.E. Jones, On the determination of molecular fields. II. From the equation of state of a gas. Proc. R. Soc. 106, 463–477 (1924)
38. J.A. Kunc, Transport integrals $\Psi(T)$ for binary collisions of open-shell atoms with uncertain interaction potentials. Phys. Rev. E 58, 4960–4966 (1998)
39. L.V. Woodcock, Equation of state for the viscosity of Lennard–Jones fluids. AIChE J. 52, 438–446 (2006)
40. B.E. Poling, J.M. Prausnitz, J.P. O’Connell, The Properties of Gases and Liquids, 5th edn. (Mc Graw Hill, Boston, 2007)
41. M. Thol, G. Rutkai, A. Köster, R. Lustig, R. Span, J. Vrabec, Equation of state for the Lennard–Jones fluid. J. Phys. Chem. Ref. Data 45, 023101 (2016)
42. C. Bannwarth, E. Caldeweyher, S. Ehrlert, A. Hansen, P. Pracht, J. Seibert, S. Spicher, S. Grimme, Extended tight-binding quantum chemistry methods. WIREs Comput. Mol. Sci. 11, 1493 (2021)
43. Wolfram Research Inc.: Mathematica, Version 13.0.0 (Champaign, 2021). https://www.wolfram.com/mathematica.
44. I.N. Ivchenko, S.K. Loyalka, R.V.J. Tompson, Analytical Methods for Problems of Molecular Transport (Springer, Dordrecht, 2007)
45. A. Laesecke, C.D. Muzny, Reference correlation for the viscosity of carbon dioxide. J. Phys. Chem. Ref. Data 46, 013107 (2017)
46. T.R. Marrero, E.A. Mason, Gaseous diffusion coefficients. J. Phys. Chem. Ref. data 1, 3–118 (1972)
47. L. Zarkova, U. Hohm, M. Damyanova, Comparison of Lorentz-Berthelot and Tang-Toennies mixing rules using an isotropic temperature-dependent potential applied to the thermophysical properties of binary gas mixtures of CH₄, CF₄, SF₆, and C(CH₃)₄ with Ar, Kr, and Xe. Int. J. Thermophys. 25, 1775–1798 (2004)
48. M. Damyanova, L. Zarkova, U. Hohm, Effective intermolecular interaction potentials of gaseous fluorine, chlorine, bromine, and iodine. Int. J. Thermophys. 30, 1165–1178 (2009)
49. L. Zarkova, U. Hohm, $pVT$ second virial coefficients $B(T)$, viscosity $\eta(T)$, and self-diffusion $D(T)$ of the gases: BF₃, CF₃, SiF₄, CCl₄, SiCl₄, SF₆, MoF₆, WF₆, UF₆, C(CH₃)₄, and Si(CH₃)₄ determined by means of an isotropic temperature-dependent potential. J. Phys. Chem. Ref. Data 31, 183–216 (2002)
50. L. Zarkova, U. Hohm, M. Damyanova, Viscosity, second $pVT$-virial coefficient, and diffusion of pure and mixed small alkanes CH₄, C₂H₆, C₃H₈, n-C₄H₁₀, n-C₅H₁₂, i-C₅H₁₂, and C(CH₃)₄ calculated by means of an isotropic temperature-dependent potential. I. Pure alkanes. J. Phys. Chem. Ref. Data 35, 1331–1364 (2006)
51. J. Kestin, K. Kneriem, E.A. Mason, B. Najafi, S.T. Ro, M. Waldman, Equilibrium and transport properties of the noble gases and their mixtures at low density. J. Phys. Chem. Ref. Data 13, 229–303 (1984)

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