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**Ab initio potential energy curve for the neon atom pair and thermophysical properties for the dilute neon gas. II. Thermophysical properties for low-density neon**

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***Ab initio* potential energy curve for the neon atom pair and  
thermophysical properties for the dilute neon gas.**

**II. Thermophysical properties for low-density neon**

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A neon-neon interatomic potential energy curve determined from quantum-mechanical *ab initio* calculations and described with an analytical representation (R. Hellmann, E. Bich, and E. Vogel, *Molec. Phys.* (in press)) was used in the framework of the quantum-statistical mechanics and of the corresponding kinetic theory to calculate the most important thermophysical properties of neon governed by two-body and three-body interactions. The second and third pressure virial coefficients as well as the viscosity and thermal conductivity coefficients, the last two in the so-called limit of zero density, were calculated for natural Ne from 25 K to 10,000 K. Comparison of the calculated viscosity and thermal conductivity with the most accurate experimental data at ambient temperature shows that these values are accurate enough to be applied as standard values for the complete temperature range of the calculations characterized by an uncertainty of about  $\pm 0.1\%$  except at the lowest temperatures.

*Keywords:* Neon pair potential; neon gas property standards; second and third pressure virial coefficients; viscosity; thermal conductivity.

## 1 Introduction

Recently we calculated standard values for some thermophysical two-body and three-body properties of helium over the temperature range from 1 K to 10,000 K with uncertainties that are superior to experimental data [1]. Prerequisite for it was the determination of a state-of-the-art pair potential between two helium atoms [2]. In order to establish a second standard for the calibration of high-precision measuring instruments at low density, we developed very recently a new interatomic pair potential for neon from high-level supermolecular *ab initio* calculations for a large number of internuclear separations  $R$  (paper I [3]). The *ab initio* calculated interatomic potential energy values  $V(R)$ , including core-core and core-valence correlation and relativistic corrections as well as coupled-cluster contributions up to

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CCSDT(Q), were listed in Table 2 of paper I. They were used for the fit of an analytical potential function, which represents a modification of the potential function given by Tang and Toennies [4]:

$$V(R) = A \exp(a_1 R + a_2 R^2 + a_{-1} R^{-1} + a_{-2} R^{-2}) - \sum_{n=3}^8 \frac{C_{2n}}{R^{2n}} \left[ 1 - \exp(-bR) \sum_{k=0}^{2n} \frac{(bR)^k}{k!} \right]. \quad (1)$$

Whereas the details of the fit were communicated in paper I, the potential parameters are repeated here for convenience in Table 1.

A comparison in paper I with experimental rovibrational spectra [5] showed that the new potential function is superior to the *ab initio* potential by Cybulski and Toczyłowski [6]. This potential was given as an analytical function derived from *ab initio* values calculated for a large range of internuclear distances. Furthermore, the comparison made evident that our new potential is at least as good as the best semi-empirical potential by Aziz and Slaman [7] and also compares well with the potential of Wüest and Merkt [5] fitted directly to the rovibrational spectra under discussion. It is noteworthy that the rovibrational spectra are sensitive to the shape of the potential well. Hence it could be possible that the potential of Wüest and Merkt is not so effective with respect to other regions of the potential. On the contrary, the transport properties are particularly sensitive to the repulsive part of the potential. Thus the potential of Aziz and Slaman could be expected to perform well in nearly all regions of the potential, since it was determined in a fit to high-energy beam data and to viscosity coefficients, considering calculated values of the  $C_6$ ,  $C_8$  and  $C_{10}$  dispersion coefficients.

In this paper we report standard values of the second and third pressure virial coefficients as well as of the viscosity and thermal conductivity coefficients in the limit of zero density for neon in its natural isotopic composition. Even though the quality of the new neon *ab initio* potential of paper I [3] is somewhat inferior compared with our recent *ab initio* potential for helium [2], the calculated thermophysical properties are expected to be as accurate as the best experimental measurements at room temperature and more accurate than available experimental data far above and far below room temperature. In order to assess as accurately as possible the quality of the potentials considered in this paper, some of the experimental viscosity data from the literature were recalibrated with reference values derived from the new interatomic potential for helium [1, 2].

## 2 Quantum-mechanical calculation of thermophysical properties

### 2.1 Evaluation of the phase shifts

A quantum-mechanical treatment of the elastic scattering is needed to obtain very accurate values for the thermophysical properties of neon. For this purpose the relative phase shifts  $\delta_l(k)$  have to be evaluated as asymptotic limiting values of the relative phases of the perturbed and unperturbed radial factor wave functions  $\psi_l(R)$  and  $\psi_l^{(0)}(R)$  (the latter with  $V(R) = 0$ ). Each of them corresponds to a particular state of the angular momentum of the system characterized by the quantum number  $l$ . To obtain the relative phase shifts  $\delta_l(k)$ , the Schrödinger equation is to be solved by numerical integration for many values of the wave number  $k = (2\mu E)^{1/2}/\hbar$ , where  $E$  is the energy of the incoming wave and  $\mu = (m_1 m_2)/(m_1 + m_2)$  is the reduced mass.

In principle, neon is to consider as a mixture of the three isotopes  $^{20}\text{Ne}$ ,  $^{21}\text{Ne}$ , and  $^{22}\text{Ne}$  with the relative atomic masses 19.9924356, 20.9938428, and 21.9913831, with the nuclear spins  $s$  of 0, 3/2, and 0, and with the natural abundances 90.48 atom%, 0.27 atom%, and 9.27 atom%. Hence there are six different interacting systems in naturally occurring neon with varying reduced masses and different statistics:  $^{20}\text{Ne}$ - $^{20}\text{Ne}$  and  $^{22}\text{Ne}$ - $^{22}\text{Ne}$  (both Bose-Einstein statistics),  $^{21}\text{Ne}$ - $^{21}\text{Ne}$  (Fermi-Dirac statistics),  $^{20}\text{Ne}$ - $^{21}\text{Ne}$ ,  $^{20}\text{Ne}$ - $^{22}\text{Ne}$ , and  $^{21}\text{Ne}$ - $^{22}\text{Ne}$  (all Boltzmann statistics). As a consequence, the relative phase shifts have to be calculated for these six binary systems at a multiplicity of wave numbers  $k$  or of energies  $E$  for a substantial number of  $l$  values which requires plenty of computing time. In order to save time the semi-classical JWKB method was used as approximation. Problems and the procedure of the fully quantum-mechanical calculation as well as the JWKB method for the determination of the relative phase shifts were discussed in some detail in our paper on helium [1].

To avoid uncertainties in the results of the calculated thermophysical properties, a very large number of phase shifts  $\delta_l(k)$  was determined for 500 values of the energy  $E$  from zero to about 135,000 K and for an increasing number of  $l$  values related to the energy. The calculations of the phase shifts were first performed fully quantum-mechanically and for comparison parallel to it according to the JWKB approximation. If the values resulting from both procedures became practically identical for certain values of the angular momentum quantum number  $l$ , the fully quantum-mechanical evaluation (QM) was finished and substituted by the semi-classical JWKB procedure at the higher  $l$  values. Table 2 gives an overview about the number of phase shifts determined for some reduced energies  $E^* = E/\varepsilon$ .

## 2.2 Calculation of the second and third pressure virial coefficients

In this paper two alternative ways were used to calculate the second virial coefficient of naturally occurring neon as a function of temperature  $T$ . In the first variant  $B(T)$  is determined like that of a mixture composed of the three neon isotopes:

$$B_{\text{mix}}(T) = \sum_{i=1}^3 \sum_{j=1}^3 x_i x_j B_{ij}(T), \quad (2)$$

whereas the second virial coefficients  $B_{ij}$  are evaluated fully quantum-mechanically for the different statistics using two contributions  $B_{\text{direct}}$  and  $B_{\text{exch}}$  [8]. In the Boltzmann statistics (B) the second virial coefficient is given as

$$B_B = B_{\text{direct}}, \quad (3)$$

whereas for particles with spin quantum number  $s$  according to the Bose-Einstein (BE) or to the Fermi-Dirac (FD) statistics holds:

$$B_{\text{BE}} = B_{\text{direct}} + B_{\text{exch}}, \quad (4)$$

$$B_{\text{FD}} = B_{\text{direct}} - B_{\text{exch}}. \quad (5)$$

$B_{\text{direct}}$  and  $B_{\text{exch}}$  result from summations over the angular momentum quantum number  $l$ , either over only the even  $l$  values or over only the odd  $l$  values:

$$B_{\text{direct}} = B_{\text{even}} + B_{\text{odd}}, \quad (6)$$

$$B_{\text{exch}} = \left( \frac{1}{2s+1} \right) \left( B_{\text{even}} - B_{\text{odd}} - \frac{N_A \Lambda^3}{16} \right). \quad (7)$$

The spin quantum numbers  $s$  and the statistics have already been given in Section 2.1 for the six interacting systems composed of the three neon isotopes. The summations over  $l$  are represented by:

$$B(T) = -\frac{N_A \Lambda^3}{2} \left[ \sum_{n=0}^{n_{\text{max}}} \sum_l^{l_{\text{max}}(n)} (2l+1) \left( e^{-\beta E_{nl}^-} - 1 \right) + \int_0^\infty \sum_l^\infty (2l+1) \frac{\delta_l(E)}{\pi} e^{-\beta E} d(\beta E) \right]. \quad (8)$$

Here  $\Lambda$  is the thermal wave length:

$$\Lambda = \left( \frac{h^2 \beta}{2\pi \mu} \right)^{\frac{1}{2}}, \quad \beta = \frac{1}{k_B T}, \quad (9)$$

whereas  $h$  is Planck's constant and  $N_A$  is Avogadro's number. The first term of Eq. (8) corresponds to the contribution of the bound states, where  $E_{nl}^-$  is the nega-

1 tive eigenvalue of the  $n$ th vibrational state with the angular-momentum quantum  
 2 number  $l$  which is obtained from the solution of the Schrödinger equation for the  
 3 radial factor wave functions  $\psi_l(R)$ . Some bound states corresponding to the ro-  
 4 tational levels for the three vibrational states of the ground electronic state of  
 5 the  $^{20}\text{Ne}$ - $^{20}\text{Ne}$  and  $^{20}\text{Ne}$ - $^{22}\text{Ne}$  dimers were listed for the neon-neon interatomic  
 6 potential under discussion in Tables 4 and 5 of our paper I [3]. The bound states  
 7 contribution is particularly of importance at low temperatures. The second term of  
 8 Eq. (8) is the essential contribution at medium and higher temperatures and is re-  
 9 lated to the scattering resulting from binary collisions and to the phase shifts  $\delta_l(E)$ .  
 10 Due to the fact that the sum over  $l$  and the integral in Eq. (8) have limits from 0  
 11 to  $\infty$ , serious errors in the computation may occur when truncated inadequately.  
 12 Therefore, it was verified that the energies for which the evaluation was performed  
 13 and particularly the number of the phase shifts were chosen large enough.

14 In the second variant naturally occurring neon is considered as a pure gas con-  
 15 sisting of atoms with the average relative atomic mass 20.1797. Then the second  
 16 virial coefficient  $B(T)$  is derived as the sum of a classical contribution as well as  
 17 of first-order, second-order, and third-order quantum corrections [9]:

$$27 \quad B(T) = B_{\text{cl}}(T) + \lambda B_{\text{qm},1}(T) + \lambda^2 B_{\text{qm},2}(T) + \lambda^3 B_{\text{qm},3}(T) + \dots \quad (10)$$

28 with  $\lambda = \frac{\hbar^2 \beta}{12m}$  and  $\hbar = \frac{h}{2\pi}$ . The individual summands are given as:

$$30 \quad B_{\text{cl}}(T) = -2\pi N_A \int_0^\infty [e^{-\beta V(R)} - 1] R^2 dR, \quad (11)$$

$$32 \quad B_{\text{qm},1}(T) = 2\pi N_A \int_0^\infty [\beta V'(R)]^2 e^{-\beta V(R)} R^2 dR, \quad (12)$$

$$34 \quad B_{\text{qm},2}(T) = -2\pi N_A \int_0^\infty \left\{ \frac{6}{5} [\beta V''(R)]^2 + \frac{12}{5R^2} [\beta V'(R)]^2 + \frac{4}{3R} [\beta V'(R)]^3 \right. \\ 36 \quad \left. - \frac{1}{6} [\beta V'(R)]^4 \right\} e^{-\beta V(R)} R^2 dR, \quad (13)$$

$$38 \quad B_{\text{qm},3}(T) = 2\pi N_A \int_0^\infty \left\{ \frac{36}{35} [\beta V'''(R)]^2 + \frac{216}{35R^2} [\beta V''(R)]^2 + \frac{24}{21} [\beta V''(R)]^3 \right. \\ 40 \quad + \frac{24}{5R} [\beta V'(R)] [\beta V''(R)]^2 + \frac{288}{315R^3} [\beta V'(R)]^3 - \frac{6}{5} [\beta V'(R)]^2 [\beta V''(R)]^2 \\ 42 \quad \left. - \frac{2}{15R^2} [\beta V'(R)]^4 - \frac{2}{5R} [\beta V'(R)]^5 + \frac{1}{30} [\beta V'(R)]^6 \right\} e^{-\beta V(R)} R^2 dR. \quad (14)$$

44 For the evaluation of the third pressure virial coefficient  $C(T)$ , naturally occur-  
 45 ing neon is again assumed to be a pure gas composed of atoms with the same

mass. Furthermore,  $C(T)$  is calculated as a sum of three contributions [10, 11], one term for the pairwise additivity of the two-body interatomic potentials  $C_{\text{add}}$ , an extra genuine term  $C_{\text{non-add}}$  for the non-additivity  $\Delta V_3(R_{12}, R_{13}, R_{23})$  of the three-body interatomic interaction potential  $V_3(R_{12}, R_{13}, R_{23})$ , and a first-order correction term for the quantum effects  $C_{\text{qm},1}$ :

$$C(T) = C_{\text{add}}(T) + C_{\text{non-add}}(T) + \lambda C_{\text{qm},1}(T) + \dots \quad (15)$$

The formulas for the three contributions have already been given in our paper on helium [1] so that it is not necessary to repeat the details. Here the only difference consists in that  $\lambda = \frac{\hbar^2 \beta}{12m}$  is separated in the first-order correction term of the quantum effects  $C_{\text{qm},1}$ . The non-additivity contribution  $\Delta V_3(R_{12}, R_{13}, R_{23})$  to the three-body potential is again approximated by the Axilrod-Teller triple-dipole potential term [12, 13], in which the non-additivity coefficient of the triple-dipole term calculated for neon by Kumar and Meath [14],  $C_9 = 1.228 \times 10^{-5} \text{ K (nm)}^9$ , is used.

### 2.3 Calculation of the transport properties

Different alternative ways were used to determine the transport properties of naturally occurring neon as a function of temperature  $T$ . In the first variant  $\eta(T)$  and  $\lambda(T)$  are evaluated quantum-mechanically and approximately like that of a dilute-gas mixture in the limit of zero density composed of the three neon isotopes. In the first-order approximation of the kinetic theory the viscosity is formulated as:

$$[\eta_{\text{mix}}]_1 = \frac{\begin{vmatrix} H_{11} & H_{12} & H_{13} & x_1 \\ H_{21} & H_{22} & H_{23} & x_2 \\ H_{31} & H_{32} & H_{33} & x_3 \\ x_1 & x_2 & x_3 & 0 \end{vmatrix}}{\begin{vmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{vmatrix}}, \quad (16)$$

$$H_{ij} = 2x_i m_i \sum_{k=1}^3 \frac{x_k m_k}{[\eta_{ik}]_1 (m_i + m_k)^2} \left[ \frac{5}{3A_{ik}} (\delta_{ij} - \delta_{jk}) + \frac{m_k}{m_i} \delta_{ij} + \delta_{jk} \right], \quad (17)$$

$$[\eta_{ij}]_1 = \frac{5}{16} \frac{(2\pi \mu_{ij} k_B T)^{1/2}}{\Omega_{ij}^{(2,2)}(T)}, \quad (18)$$

$$A_{ik} = \frac{\Omega_{ik}^{(2,2)}(T)}{\Omega_{ik}^{(1,1)}(T)}, \quad \mu_{ij} = \frac{m_i m_j}{m_i + m_j}. \quad (19)$$



The symbol  $[\eta_{ij}]_1$  represents the first-order approximation of the viscosity characterizing the interaction between a binary pair  $i$ - $j$ . Here all different  $[\eta_{ij}]_1$  are given in terms of collision integrals  $\Omega_{ij}^{(2,2)}(T)$  which have to be evaluated quantum-mechanically (see below).  $\delta_{ij}$  is the Kronecker symbol,  $A_{ik}$  corresponds to the ratio of two collision integrals, whereas  $\mu_{ij}$  is the reduced mass of the interacting pair.

In analogy to Eq. (16) an equation in which the elements  $H_{ij}$  are replaced by elements  $L_{ij}$  is applied for the thermal conductivity of a dilute gas mixture in its first-order approximation. The elements  $L_{ij}$  are expressed as:

$$L_{ij} = x_i m_i \sum_{k=1}^3 \frac{x_k m_k}{[\lambda_{ik}]_1 (m_i + m_k)^2} \left\{ \frac{5}{8A_{ik}^*} \left[ \left( 6 \frac{m_i}{m_k} + 5 \frac{m_k}{m_i} \right) \delta_{ij} - 11 \delta_{jk} \right] - \frac{3B_{ik}}{2A_{ik}} \left( \frac{m_k}{m_i} \delta_{ij} - \delta_{jk} \right) + 2(\delta_{ij} + \delta_{jk}) \right\}, \quad (20)$$

$$[\lambda_{ij}]_1 = \frac{75 (2\pi\mu_{ij}k_B^3 T)^{1/2}}{64 \cdot 2\mu_{ij}\Omega_{ij}^{(2,2)}(T)}, \quad (21)$$

$$B_{ik} = \frac{5\Omega_{ik}^{(1,2)}(T) - 4\Omega_{ik}^{(1,3)}(T)}{\Omega_{ik}^{(1,1)}(T)}. \quad (22)$$

Here  $[\lambda_{ij}]_1$  is the first-order approximation of the thermal conductivity related to the interaction between a binary pair  $i$ - $j$  and again given in terms of the  $\Omega_{ij}^{(2,2)}(T)$  collision integrals.  $B_{ik}$  represents a relation between different collision integrals.

In principle, exact calculations require higher-order approximations of the kinetic theory. Therefore, we used fifth-order approximations in the case of the transport properties of helium [1], but the calculations for  $^3\text{He}$  and  $^4\text{He}$  concerned a pure gas each. Unfortunately, approximations of such a high order are not available for mixtures so that we were forced to choose any other reasonable way for the higher-order calculations of the transport properties of naturally occurring neon and tested thus two possibilities. On the one hand, the individual viscosity and thermal conductivity coefficients  $\eta_{ij}$  and  $\lambda_{ij}$  for the binary pairs with like and unlike interactions are calculated up to the fifth-order approximation according to:

$$[\eta_{ij}]_5 = \frac{5}{16} \frac{(2\pi\mu_{ij}k_B T)^{1/2}}{\Omega_{ij}^{(2,2)}(T)} f_{\eta,ij}^{(5)}, \quad (23)$$

$$[\lambda_{ij}]_5 = \frac{75}{64} \frac{(2\pi\mu_{ij}k_B^3 T)^{1/2}}{2\mu_{ij}\Omega_{ij}^{(2,2)}(T)} f_{\lambda,ij}^{(5)}. \quad (24)$$

Here  $f_{\eta,ij}^{(5)}$  and  $f_{\lambda,ij}^{(5)}$  represent the correction factors for the fifth-order approximations of the kinetic theory. The resulting values for  $[\eta_{ij}]_5$  and  $[\lambda_{ij}]_5$  are then used in the first-order approximation for the mixture viscosity represented by Eq. (16) as well as in the corresponding relation for the thermal conductivity. On the other

hand, the values of the first-order approximations  $[\eta_{\text{mix}}]_1$  [Eq.(16)] and  $[\lambda_{\text{mix}}]_1$  are corrected for the fifth-order approximations by means of correction factors  $f_{\eta}^{(5)}$  and  $f_{\lambda}^{(5)}$ . These are derived using collision integrals which are also determined quantum-mechanically for a pure neon gas consisting of atoms with the average relative atomic mass 20.1797 and following the Bose-Einstein statistics for  $^{20}\text{Ne}$ – $^{20}\text{Ne}$ . For the calculations of  $f_{\eta,ij}^{(5)}$  and  $f_{\lambda,ij}^{(5)}$  as well as  $f_{\eta}^{(5)}$  and  $f_{\lambda}^{(5)}$  we used explicit expressions and computer programs provided by Viehland et al. [15]. According to our calculations the effect of the fifth-order corrections to the viscosity and to the thermal conductivity compared with the fourth-order corrections is below  $\pm 0.01\%$ .

Expressions for the quantum cross sections  $Q^{(m)}(E)$  and for the quantum collision integrals  $\Omega^{(m,s)}(T)$  needed in the different approximations of the solution of the Boltzmann equation were derived by Meeks et al. [16]. They were again collected in our paper for helium [1] for particles with spin  $s$  according to the Bose-Einstein (BE) or to the Fermi-Dirac (FD) statistics as well as for the Boltzmann statistics. The formulas for the different  $Q^{(m)}$  are related to sums over the phase shifts  $\delta_l$ , either over only the odd  $l$  values or over only the even  $l$  values, but also over complete sums (Boltzmann statistics). The quantum collision integrals  $\Omega^{(m,s)}(T)$  result from the quantum cross sections  $Q^{(m)}(E)$  according to:

$$\Omega^{(m,s)}(T) = \frac{4\pi\hbar^2}{2\mu k_{\text{B}}T(s+1)!} \int_0^{\infty} Q^{(m)}(E) e^{-\beta E} (\beta E)^s d(\beta E). \quad (25)$$

In a second variant the viscosity of neon was determined classically for the first-order and the fifth-order approximations in order to examine whether a quantum-mechanical calculation is actually needed to achieve highly accurate values for the transport properties of neon in the zero-density limit. For this purpose the usual formulations for monatomics [17] were used, whereas neon was again considered to be a pure gas with the average relative atomic mass already given.

### 3 Comparison with experimental data and values for other interatomic potentials

#### 3.1 Second and third pressure virial coefficients

The quantum-mechanical calculation of the second pressure virial coefficient requires the determination of the existing bound states. For this purpose the Level 7.7 program of LeRoy [18] was used. As already mentioned in Section 2.2, the bound states of the  $^{20}\text{Ne}$ – $^{20}\text{Ne}$  and  $^{20}\text{Ne}$ – $^{22}\text{Ne}$  dimers were listed in our paper I [3] in which they were compared with the experimental rovibrational spectra by Wüest and Merkt [5].

In figure 1 the values calculated fully quantum-mechanically for the interatomic potential of the present paper are opposed to those resulting from quantum cor-

rections of increasing order added to the classical contribution. The figure illustrates that the classical contribution alone is completely insufficient to describe adequately the second pressure virial coefficient. The agreement between both ways of calculation improves with the quantum corrections included what becomes obvious particularly at low temperatures. To obtain close agreement even at the lowest temperatures, the third-order quantum correction is needed.

There exists only a limited number of experimental data for second and third pressure virial coefficients of neon in the literature compared with those of common gases like argon and nitrogen as well as with those of helium. Furthermore, it is to point out that experimental data for the third pressure virial coefficient are not independent of the values for the second pressure virial coefficient derived from the same experiments. Hence third pressure virial coefficients combined with second ones are included in the comparison. Second and third pressure virial coefficients were determined by Holborn and Otto [19], Nicholson and Schneider [20], Michels et al. [21], and Gibbons [22] from isothermal measurements of volume (and density, respectively) and pressure. Vogl and Hall [23] used a Burnett apparatus to derive isothermal compression factors and to obtain finally second and third pressure virial coefficients. **Unfortunately, in none of these papers an error propagation analysis or uncertainties of the second and third pressure virial coefficients adequately deduced from the experiments were reported.**

The experimental  $B$  data are compared with the values calculated fully quantum-mechanically for the neon–neon interatomic potential of the present paper in figure 2, in which the absolute deviations  $B_{\text{exp}} - B_{\text{cal(pres)}}$  are displayed. The figure demonstrates a very good agreement for the excellent data by Michels et al. [21] at medium temperatures. A good agreement is also found for the data by Nicholson and Schneider [20] up to high temperatures of 1,000 K. On the contrary, the very old data of Holborn and Otto [19] as well as the more recent but also already 35 years old data of Vogl and Hall [23] are characterized by comparably larger differences to the theoretically calculated values. The data of Gibbons [22] determined at low temperatures show partly large deviations, but agree partly very well. In figure 2 our calculated values are additionally compared with the values calculated for the interatomic potentials by Aziz and Slaman [7], Cybulski and Toczyłowski [6], and Wüest and Merkt [5]. The differences  $B_{\text{cal(lit)}} - B_{\text{cal(pres)}}$  derived for the different interatomic potentials increase to low temperatures, where the values derived from the potentials by Aziz and Slaman [7] and Wüest and Merkt [5] are too small and the values resulting from the potential by Cybulski and Toczyłowski [6] are too large. At medium and higher temperatures the  $B_{\text{cal}}$  values for all four potentials do not differ much so that the second pressure virial coefficient is not suitable to distinguish between the different interatomic potentials.

In figure 3 a comparison between experimental data of the third pressure virial

1 coefficient of neon and values calculated for the new interatomic potential is shown.  
2 The figure elucidates that good agreement of the experimental data by Michels et al.  
3 [21] and by Nicholson and Schneider [20] at medium temperatures and of the data  
4 by Gibbons [22] at low temperatures with the calculated values is only achieved  
5 in the case of the complete sum of the contributions for the pairwise additivity  
6  $C_{\text{add}}$ , for the non-additivity of the three-body interatomic interactions according to  
7 Axilrod and Teller  $C_{\text{non-add}}$ , and for the first-order quantum-mechanical correction  
8  $\lambda C_{\text{qm},1}$ . The experimental data by Holborn and Otto [19] as well as Vogl and  
9 Hall [23] possess again larger differences to the calculated values. The comparison  
10 makes evident that the calculation procedure for the third pressure virial coefficient  
11 predicts very good values.  
12

13 It is to be stressed that the calculated values for the second and the third pressure  
14 virial coefficients are more reliable than the experimental data at low and high  
15 temperatures.  
16

### 17 3.2 Viscosity

18 First, the results of the different alternative ways of the calculation of the transport  
19 properties of naturally occurring neon are compared. In this context it is sufficient  
20 to consider only the viscosity, since the effects are the same for the thermal conduc-  
21 tivity. Figure 4 illustrates the relative differences between viscosity values derived  
22 for the different approximation procedures and the viscosity values obtained from  
23 the quantum-mechanical calculation up to the fifth-order approximation for the in-  
24 dividual  $[\eta_{ij}]_{\text{qm},5}$  within the first-order formulation of  $[\eta_{\text{mix}}]_1$  (see Section 2.3). The  
25 figure makes evident that the first-order approximation of the classical calculation  
26 leads to values which are nearly 1% too small in the complete temperature range  
27 except at the lowest temperatures. The agreement improves when the fifth-order  
28 approximation of the classical evaluation is applied. But even for this high-order  
29 approximation it becomes obvious that the classical evaluation is not appropriate  
30 with regard to highly accurate values. Thus the deviations from the results for the  
31 quantum-mechanical calculation of the same fifth-order approximation amount to  
32  $-0.1\%$  at room temperature increasing up to  $-1.1\%$  at about 60 K. On the other  
33 hand, the first-order approximation of the quantum-mechanical calculation for a  
34 dilute-gas mixture composed of the three neon isotopes according to  $[\eta_{\text{mix}}]_{\text{qm},1}$  is  
35 not adequate, too. The differences are approximately  $-0.7\%$  at most temperatures  
36 and decrease to zero at the lowest temperatures. Further it is to note that there  
37 are only differences of  $< \pm 0.0004\%$  (not visible in figure 4) between the results for  
38 the two ways to correct the first-order approximation  $[\eta_{\text{mix}}]_{\text{qm},1}$  to an appropriate  
39 fifth-order approximation of the quantum-mechanical determination. In the follow-  
40 ing the comparisons with experimental data are performed with values resulting  
41 for the fifth-order approximation of the individual  $[\eta_{ij}]_{\text{qm},5}$  and  $[\lambda_{ij}]_{\text{qm},5}$  within the  
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1 first-order formulations of  $[\eta_{\text{mix}}]_1$  and  $[\lambda_{\text{mix}}]_1$ .

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3 With regard to the transport properties it is to consider that most measurements  
4 at low densities were performed at atmospheric pressure, whereas the theoretical  
5 calculations are valid for the limit of zero density. Hence the initial density depen-  
6 dence of the experimental data would have to be taken into account. However apart  
7 from the very low temperatures near to the normal boiling point of neon, the effect  
8 of the initial density dependence on the transport properties concerning the change  
9 in density from that at atmospheric pressure to zero density is comparably small  
10 ( $< 0.1\%$ ) for all other temperatures. Furthermore, the experimental uncertainty is  
11 distinctly increased at low temperatures.

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15 In our paper concerning the thermophysical standard values for low-density he-  
16 lium [1] we argued that it is difficult to perform genuine absolute measurements  
17 of the gas viscosity with an uncertainty  $< \pm 0.1\%$ , even at room temperature. The  
18 same complex of problems is illustrated in figure 5 in which the best experimental  
19 data for neon near to ambient temperature are characterized by error bars for the  
20 uncertainties, given by the authors themselves, and are compared with the viscos-  
21 ity values calculated quantum-mechanically. For helium we demonstrated that the  
22 measurements with an oscillating-disk viscometer by Kestin and Leidenfrost [24],  
23 approved as one of the most accurate and additionally one of the few absolute mea-  
24 surements on gases, can only partly be considered as absolute ones, since they were  
25 finally adjusted to a value for the viscosity of air at 293.15 K and at atmospheric  
26 pressure determined by Bearden [31] in an absolute measurement with a rotating-  
27 cylinder viscometer. Thus the viscosity value of Kestin and Leidenfrost for neon  
28 at 20°C (uncertainty:  $\pm 0.05\%$ ) shown in figure 5 corresponds as well to a relative  
29 measurement, whereas the genuine absolute measurement is that of Bearden on  
30 air. Measurements by Kestin and Nagashima [25], performed in a nearly analogous  
31 procedure, led to values which are 0.15–0.3% higher than those of Kestin and Lei-  
32 denfrost [24], but also by the same percentage higher than further data obtained  
33 in relative measurements of the same research group by DiPippo et al. [26] as well  
34 as a best estimate reported by Kestin et al. [27] in 1972 as a result of their mea-  
35 surements in foregoing years. This shows that there were sometimes surprisingly  
36 large differences in the results of the measurements of this group. Nevertheless,  
37 the results of the most reliable measurements by Kestin and co-workers at am-  
38 bient temperature are characterized by a tendency to values increased by +0.1%  
39 compared to the calculated values of the present paper. The same findings con-  
40 cerning the measurements by Kestin and co-workers were observed in the case of  
41 the values derived from our interatomic helium potential. As a consequence, the  
42 measurements on helium by Vogel [29] (uncertainty:  $\pm 0.15\%$  at room temperature)  
43 performed with an all-quartz oscillating-disk viscometer in a relative manner using  
44 a viscometer constant derived from the best estimate by Kestin et al. should be  
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1 affected by the same impact. Therefore, the viscometer of Vogel was recalibrated  
2 with the new helium standard for a rehandled evaluation of the measurements on  
3 helium [1] and on neon, too. The influence of the recalibration on the results of  
4 Vogel [1] and on neon, too. The influence of the recalibration on the results of  
5 Vogel for neon is additionally demonstrated in figure 5. A value at 298.15 K result-  
6 ing from the fitting function given by Vogel [29] deviates from the value calculated  
7 for the interatomic neon potential of the present paper by +0.18%. On the con-  
8 trary, the direct experimental data of the measurement series by Vogel at room  
9 temperature show only differences of +0.04% and +0.08% after the recalibration.

10 Furthermore, the absolute measurements by Flynn et al. [28] performed with a  
11 capillary viscometer led to a datum at 293.15 K differing only by +0.01% from the  
12 theoretically calculated value (uncertainties:  $\pm 0.1\%$ ). Recently, Evers et al. [30]  
13 utilized a rotating-cylinder viscometer for absolute measurements (uncertainty:  
14  $\pm 0.15\%$ ) on several gases at different temperatures and pressures. Their result for  
15 neon at 298.15 K deviates from our calculated value by  $-0.12\%$ . In conclusion, the  
16 comparison makes evident that the best experimental data at room temperature are  
17 characterized by an uncertainty of  $\pm(0.1 \text{ to } 0.15)\%$  and that they agree within this  
18 limit with the values calculated for the interatomic neon potential of the present  
19 paper.  
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21 The situation deteriorates to the disadvantage of the experiment, if the mea-  
22 surements were not performed at ambient temperature. In figure 6, experimental  
23 data at low and medium temperatures between 20 K and 373 K are compared with  
24 the calculated values. Error bars for one or two (in the case that the uncertainty  
25 changes with temperature) values of each data set are additionally plotted. The  
26 figure demonstrates that excellent agreement within  $\pm 0.1\%$  exists only for the ab-  
27 solute measurement by Evers et al. [30] at 348 K and that the results of the absolute  
28 measurements by Flynn et al. [28] are adequately consistent within  $\pm 0.3\%$ . The  
29 other data were determined by relative measurements, which are not only affected  
30 by the usual measurement errors, but also by the values used for the calibra-  
31 tion. Johnston and Grilly [32] and Rietveld et al. [34] (both using oscillating-disk  
32 viscometers) as well as Clarke and Smith [35] (capillary viscometer) based their  
33 measurements on reasonable values for air, helium, and nitrogen at ambient tem-  
34 perature and achieved results with deviations up to  $-2\%$ ,  $+4\%$ , and  $+1\%$ . These  
35 data are not suitable to judge the appropriateness of any interatomic neon poten-  
36 tial. On the other hand, the measurements by Coremans et al. [33] carried out  
37 with an oscillating-disk viscometer, which was calibrated using a very old viscosity  
38 value for  $^4\text{He}$  at 20 K reported by Kamerlingh Onnes and Weber [36], yielded val-  
39 ues characterized by positive deviations up to 6% from the quantum-mechanically  
40 calculated values. These results were improved for the purposes of this paper by a  
41 recalibration with a value for  $^4\text{He}$  at 20 K taken from our new helium standard [1].  
42 Figure 6 makes obvious that the corrected data advanced after this correction  
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1 partly in close agreement.

2 Figure 7 illustrates the analogous comparison at higher temperatures. The figure  
3 reveals a surprisingly large scattering of about  $\pm 0.3\%$  in the data from different  
4 papers by Kestin and his research group [27, 37, 38] (the same order of magni-  
5 tude as the uncertainty) and additionally a systematic trend to higher values with  
6 increasing temperature combined with again decreasing values at the highest tem-  
7 peratures. In this connection it is to note that all measurements by Kestin and his  
8 co-workers with the oscillating-disk viscometer by Di Pippo et al. [41] are affected  
9 by a temperature measurement error with thermocouples explained by Vogel et  
10 al. [42]. Figure 7 makes also evident that the data by Vogel [29], originally fit-  
11 ted to his experiments which were based on a calibration with the best estimate  
12 value at room temperature by Kestin et al. [27], deviate by about  $+0.2\%$  from the  
13 quantum-mechanically calculated values of this paper. After a recalibration of the  
14 measurement series on neon by means of the new helium standard [1] at room tem-  
15 perature, the corrected experimental data do only deviate by less than  $+0.1\%$  on  
16 average from the theoretical values for the new neon potential in the complete tem-  
17 perature range of the measurements. This demonstrates that the measurements by  
18 Vogel with his all-quartz oscillating-disk viscometer represent the best experiments  
19 in this temperature range. The comparison concerning the experimental data by  
20 Dawe and Smith [39] and by Guevara and Stensland [40], which result from rel-  
21 ative measurements with capillary viscometers based on a reasonable calibration  
22 at room temperature, shows that these data should be influenced by systematic  
23 errors. Lastly it is concluded that the theoretical determination of viscosity values  
24 is to be preferred to experiments at these high temperatures.

25 Figures 5, 6, and 7 include once again a comparison with the values derived clas-  
26 sically using the fifth-order approximation. The results of the classical calculation  
27 deviate by about  $-0.1\%$  from those of the quantum-mechanical computation at  
28 ambient and higher temperatures. At lower temperatures the deviations are dis-  
29 tinctly increased. Figure 5 elucidates further that at room temperature the results  
30 of the quantum-mechanical calculations for the potentials by Aziz and Slaman [7]  
31 and by Cybulski and Toczyłowski [6] (both  $> \pm 0.2\%$ ) and particularly by Wüest  
32 and Merkt [5] ( $-0.7\%$ , not observable in the figure) do not match the best experi-  
33 mental data as well as the calculated values for the potential of the present paper  
34 within  $\pm 0.1\%$ . Figure 6 and 7 demonstrate that the best experimental data allow to  
35 distinguish between the different potentials proposed for neon. The values resulting  
36 from the potentials by Aziz and Slaman [7] and by Cybulski and Toczyłowski [6]  
37 and particularly by Wüest and Merkt [5] are characterized by differences from the  
38 transport data that are distinctly larger than the experimental uncertainties. Here  
39 it is to point to the differences for the values determined with the potential pro-  
40 posed by Wüest and Merkt [5]. They arise with increasing temperature due to the  
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1 fact that the rovibrational spectra used by Wüest and Merkt are sensitive to the  
2 shape of the potential well, but not to the repulsive part of the potential to which  
3 the transport properties are particularly sensitive.  
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### 7 **3.3 Thermal conductivity**

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9 The uncertainty of measurements of the thermal conductivity is inferior to that  
10 of viscosity measurements due to different experimental difficulties, whereas the  
11 most accurate data can be obtained with the transient hot-wire technique, but  
12 essentially restricted to ambient temperature. This is demonstrated in figure 8, in  
13 which experimental data for neon at low and medium temperatures are compared  
14 with the values calculated quantum-mechanically. Here the experimental data are  
15 again, when available, characterized by error bars according to the uncertainties  
16 given by the experimenters themselves. The data by Kestin et al. [44] and Assael  
17 et al. [45], each gained with the transient hot-wire technique at room temperature,  
18 deviate from the calculated values by  $< -0.1\%$  and  $< +0.2\%$ . These differences  
19 are lower than the experimental uncertainties ( $\pm 0.3\%$  and  $\pm 0.2\%$ ). Although the  
20 data by Haarman [43] are characterized by larger deviations ( $-0.3\%$  to  $-0.4\%$ ),  
21 the temperature function of these transient hot-wire data between 328 K and 468 K  
22 corresponds closely to that of the calculated values. On the contrary, the tempera-  
23 ture function of the data by Millat et al. [46] shows an awkward behaviour so that  
24 these data are not useful with regard to the assessment of the values calculated  
25 for the different interatomic potentials of neon. But figure 8 makes also evident  
26 that the deviations of the experimental data of Hemminger [47], derived from  
27 measurements with a guarded parallel-plate apparatus and carefully corrected for  
28 impurities caused by desorbed air, are within  $-0.35\%$  and  $-0.6\%$ ; this means their  
29 temperature function and that of the calculated values are pretty much consistent  
30 from room temperature up to 470 K.  
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34 Experimental data determined with the common steady-state hot-wire technique  
35 often affected by convection are checked against the quantum-mechanically calcu-  
36 lated values in figure 8, too. Differences of only  $< \pm 0.4\%$  are found for the very  
37 old experimental datum by Weber [48] at 273 K and also for a value by Kannu-  
38 luik and Carman [49] at the same temperature. But for the complete temperature  
39 range of the measurements of Kannuluik and Carman between 90 K and 580 K the  
40 deviations increase up to  $-3\%$ . On the other hand, the smoothed experimental  
41 values by Nesterov and Sudnik [52] between 90 K and ambient temperature cre-  
42 ated with the same technique are characterized by comparably small differences  
43 between  $-0.1\%$  and  $-0.7\%$ , with the best agreement at low temperatures. Further  
44 it becomes evident from this figure that the experimental data by Keyes [50] deter-  
45 mined with the concentric-cylinder method (differences between  $-1\%$  and  $-1.5\%$ )  
46 and those of Sengers et al. [51] obtained with a parallel-plate apparatus (differences  
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1 between  $-0.5\%$  and  $-0.85\%$ ) are not suitable for a reasonable comparison with the  
2 theoretical values.  
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4 Figure 9 illustrates the comparison at higher temperatures. Neither the experi-  
5 mental data by Tufeu et al. [54] (concentric-cylinder method) nor the experimental  
6 values by Saxena and Saxena [53] (common hot-wire technique) enable to verify  
7 the performance of the different potentials under discussion due to the differences  
8 exceeding  $-1\%$ . On the contrary, there occur surprisingly only very small devia-  
9 tions of  $-0.45\%$  to  $+0.05\%$  for the experimental data by Springer and Wingeier [55]  
10 between 1,000 K and 1,500 K using the concentric-cylinder method. In principle,  
11 this would support the new interatomic potential of this work. In addition, the  
12 values recommended by Ziebland [56] on the basis of different experimental data  
13 show deviations larger than  $+1\%$  according to their estimated uncertainties. It is to  
14 note that thermal conductivity values at very high temperatures between 1,500 K  
15 and at most 6,000 K were derived from shock-tube measurements by Collins and  
16 Menard [57] and by Mařtovsky [58]. Their data not shown in figure 9 have devia-  
17 tions of  $-5.5\%$  up to  $-11.5\%$  and  $-2.5\%$  up to  $-6.8\%$ . At such high temperatures  
18 calculated values are to be preferred in any case.  
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20 Both figures make evident that the interatomic potential by Wüest and Merkt [5]  
21 is not qualified to describe adequately the best experimental thermal conductivity  
22 data. On the other hand, there exist only a few experimental data to distinguish  
23 between the appropriateness of the other potentials. But if the best experimental  
24 transient hot-wire-data at room temperature are selected for the comparison, then  
25 there exists a stringent test of the new potential and of the correct application of  
26 the kinetic theory including the quantum-mechanical effects.  
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#### 28 4 Summary and conclusions

29 A new interatomic potential for neon derived from quantum-mechanical *ab initio*  
30 computations [3] was utilized to calculate the second and third pressure virial, the  
31 viscosity and the thermal conductivity coefficients for dilute neon gas in its natu-  
32 ral isotopic composition in the temperature range from 25 K to 10,000 K. For the  
33 second virial coefficient and for the transport properties fully quantum-mechanical  
34 calculations were performed with neon treated as an isotopic mixture, whereas for  
35 the third virial coefficient a classical mechanical evaluation with a quantum correc-  
36 tion using the average mass of the isotopic mixture was applied. The comparison  
37 with available experimental data makes evident that the calculated thermophysical  
38 properties are as accurate as the best experimental data at room temperature and  
39 more accurate at temperatures above and below room temperature. The devia-  
40 tions between the results from the different potentials for all calculated properties  
41 increase at the lowest temperatures.  
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1 The viscosity values around ambient temperature derived theoretically with the  
2 interatomic potential of this paper are characterized by deviations smaller than  
3  $\pm 0.1\%$  compared to the best experimental data, whereas the results obtained from  
4 the potential energy curves by Cybulski and Toczyłowski, by Aziz and Slaman [7],  
5 and by Wüest and Merkt [5] show larger deviations. We estimate summarily the  
6 uncertainties of the calculated transport properties resulting from our new potential  
7 to be about  $\pm 0.1\%$  except at the lowest temperatures. It is to be stressed that this  
8 uncertainty is much below the experimental uncertainties at low as well as at high  
9 temperatures. All calculated data (see table A in the appendix) can be applied as  
10 standards values for the complete temperature range.  
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Table 1. Potential parameters

$A$	K	0.402915058383E + 08
$a_1$	(nm) <sup>-1</sup>	-0.428654039586E + 02
$a_2$	(nm) <sup>-2</sup>	-0.333818674327E + 01
$a_{-1}$	nm	-0.534644860719E - 01
$a_{-2}$	(nm) <sup>2</sup>	0.501774999419E - 02
$b$	(nm) <sup>-1</sup>	0.492438731676E + 02
$C_6$	K (nm) <sup>6</sup>	0.440676750157E - 01
$C_8$	K (nm) <sup>8</sup>	0.164892507701E - 02
$C_{10}$	K (nm) <sup>10</sup>	0.790473640524E - 04
$C_{12}$	K (nm) <sup>12</sup>	0.485489170103E - 05
$C_{14}$	K (nm) <sup>14</sup>	0.382012334054E - 06
$C_{16}$	K (nm) <sup>16</sup>	0.385106552963E - 07
$\varepsilon/k_B$	K	42.152521
$R_\varepsilon$	nm	0.30894556
$\sigma$	nm	0.27612487

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Table 2. Number of calculated phase shifts of neon for some reduced energies

$E^*$	Total number	Full QM calculation
0.	11	11
$1. \times 10^{-4}$	14	12
$1. \times 10^{-3}$	14	12
$1. \times 10^{-2}$	29	23
$5. \times 10^{-2}$	62	34
$1. \times 10^{-1}$	87	41
$5. \times 10^{-1}$	177	58
1.	244	67
3.	511	84
5.	1152	93
10.	1152	108
100.	1152	131
3,200.	1351	131

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**Fig. 1** Differences  $\Delta B = B_{\text{qm,full}} - [B_{\text{cl}} + \sum \lambda^i B_{\text{qm},i}]$  between the fully quantum-mechanically calculated values and the values resulting from the sum of a classical contribution and of different orders of quantum corrections to the second pressure virial coefficient for the new interatomic potential for Ne. Differences related to: ..... classical contribution  $B_{\text{cl}}$ ; - · - · - · sum of classical contribution and of first-order quantum correction  $B_{\text{cl}} + \lambda B_{\text{qm},1}$ ; - - - - sum of classical contribution as well as of first-order and second-order quantum corrections  $B_{\text{cl}} + \lambda B_{\text{qm},1} + \lambda^2 B_{\text{qm},2}$ ; ————— sum of classical contribution as well as of first-order, second-order, and third-order quantum corrections  $B_{\text{cl}} + \lambda B_{\text{qm},1} + \lambda^2 B_{\text{qm},2} + \lambda^3 B_{\text{qm},3}$ .

**Fig. 2** Differences  $(B - B_{\text{cal(pres)}})$  of experimental ( $B_{\text{exp}}$ ) and calculated ( $B_{\text{cal(lit)}}$ ) second pressure virial coefficients from values ( $B_{\text{cal(pres)}}$ ) calculated with the new interatomic potential for Ne. Experimental data: ○ Holborn and Otto [19]; △ Nicholson and Schneider [20]; □ Michels et al. [21]; ▽ Gibbons [22]; ◇ Vogl and Hall [23]. Calculated values: ——— potential by Aziz and Slaman [7]; - · - · - · potential by Cybulski and Toczyłowski [6]; - - - - potential by Wüest and Merkt [5].

**Fig. 3** Comparison of experimental data and of calculated values for the third pressure virial coefficient  $C$  derived from the new interatomic potential for Ne. Experimental data: ○ Holborn and Otto [19]; △ Nicholson and Schneider [20]; □ Michels et al. [21]; ▽ Gibbons [22]; ◇ Vogl and Hall [23]. Calculated values: - - - - classical contribution  $C_{\text{add}}$ , - · - · - · classical and non-additivity contributions  $C_{\text{add}} + C_{\text{non-add}}$ , ————— sum of classical and non-additivity contributions and of the first-order quantum correction  $C_{\text{add}} + C_{\text{non-add}} + \lambda C_{\text{qm},1}$ .

**Fig. 4** Relative deviations  $\Delta = 100(\eta - \eta_{\text{qm},5})/\eta_{\text{qm},5}$  between viscosity values calculated for different approximation procedures and viscosity values resulting from quantum-mechanical calculations up to the fifth-order approximation for the individual  $[\eta_{ij}]_{\text{qm},5}$  within the first-order formulation of  $[\eta_{\text{mix}}]_1$  for the new interatomic potential for Ne. Differences related to: ..... first-order classical calculation  $[\eta]_{\text{cl},1}$ ; - · - · - · fifth-order classical calculation  $[\eta]_{\text{cl},5}$ ; - · - · - · first-order quantum-mechanical calculation  $[\eta_{\text{mix}}]_{\text{qm},1}$ .

**Fig. 5** Relative deviations of experimental and calculated viscosity coefficients from values  $\eta_{\text{cal(pres)}}$  calculated quantum-mechanically with the new interatomic potential for Ne near to room temperature. Experimental data with uncertainties characterized by error bars: ● Kestin and Leidenfrost [24]; ○ Kestin and Nagashima [25]; ▼ DiPippo et al. [26]; ▽ Kestin et al. [27], best estimate; ■ Flynn et al. [28]; △ Vogel [29], fit-

ted value; ▲ Vogel [29], experimental data corrected according to new helium standard; ◆ Evers et al. [30]. Calculated values: ..... fifth-order classical calculation  $[\eta]_{cl,5}$ ; ——— potential by Aziz and Slaman [7]; - - - - - potential by Cybulski and Toczyłowski [6].

**Fig. 6** Relative deviations of experimental and calculated viscosity coefficients from values  $\eta_{cal(pres)}$  calculated with the new interatomic potential for Ne at low and medium temperatures. Experimental data **with uncertainties characterized by error bars**: □ Johnston and Grilly [32]; ○ Coremans et al. [33]; ● Coremans et al. [33], corrected according to new helium standard; △ Rietveld et al. [34]; ■ Flynn et al. [28]; ◇ Clarke and Smith [35]; ◆ Evers et al. [30]. Calculated values: ..... fifth-order classical calculation  $[\eta]_{cl,5}$ ; ——— potential by Aziz and Slaman [7]; - - - - - potential by Cybulski and Toczyłowski [6]; - - - - - potential by Wüest and Merkt [5].

**Fig. 7** Deviations of experimental and calculated viscosity coefficients from values  $\eta_{cal(pres)}$  calculated with the new interatomic potential for Ne at higher temperatures. Experimental data **with uncertainties characterized by error bars**: ▽ Kestin et al. [27], best estimate; ○ Hellemans et al. [37]; ⊙ Kestin et al. [38]; ◇ Dawe and Smith [39]; □ Guevara and Stensland [40]; △ Vogel [29], fitted values; ▲ Vogel [29], experimental data corrected according to new helium standard. Calculated values: ..... fifth-order classical calculation  $[\eta]_{cl,5}$ ; ——— potential by Aziz and Slaman [7]; - - - - - potential by Cybulski and Toczyłowski [6]; - - - - - potential by Wüest and Merkt [5].

**Fig. 8** Deviations of experimental and calculated thermal conductivity coefficients from values  $\lambda_{cal(pres)}$  calculated with the new interatomic potential for Ne at low and medium temperatures. Experimental data **with uncertainties characterized by error bars**: ● Haarman [43]; ▲ Kestin et al. [44]; ■ Assael et al. [45]; ▼ Millat et al. [46]; ◆ Hemminger [47]; ○ Weber [48]; △ Kannuluik and Carman [49]; □ Keyes [50]; ▽ Sengers et al. [51]; ◇ Nesterov and Sudnik [52], smoothed values. Calculated values: ..... fifth-order classical calculation  $[\eta]_{cl,5}$ ; ——— potential by Aziz and Slaman [7]; - - - - - potential by Cybulski and Toczyłowski [6]; - - - - - potential by Wüest and Merkt [5].

**Fig. 9** Deviations of experimental and calculated thermal conductivity coefficients from values  $\lambda_{cal(pres)}$  calculated with the new interatomic potential for Ne at higher temperatures. Experimental data **with uncertainties characterized by error bars**: ○ Saxena and Saxena [53], smoothed values; △ Tufeu et al. [54]; □ Springer and Wingeier [55]; ▽ Ziebland [56], recommended values. Calculated values: .....



1 fifth-order classical calculation  $[\eta]_{cl,5}$ ; ——— potential by Aziz and  
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3 Slaman [7]; - - - - - potential by Cybulski and Toczyłowski [6]; - -  
4 - - potential by Wüest and Merkt [5].  
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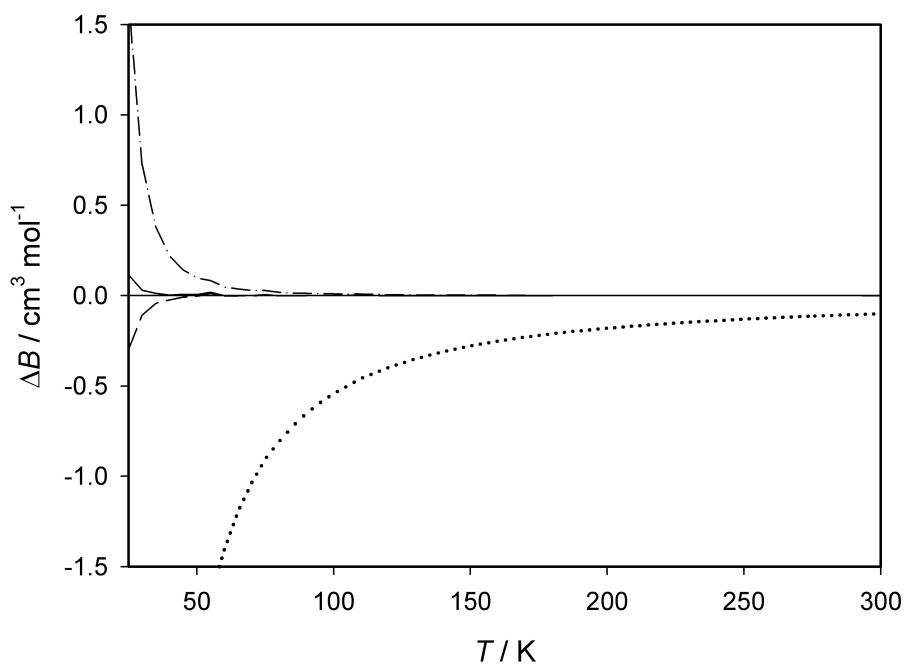


Figure 1. Differences  $\Delta B = B_{\text{qm,full}} - [B_{\text{cl}} + \sum \lambda^i B_{\text{qm},i}]$  between the fully quantum-mechanically calculated values and the values resulting from the sum of a classical contribution and of different orders of quantum corrections to the second pressure virial coefficient for the new interatomic potential for Ne. Differences related to:  $\dots\dots\dots$  classical contribution  $B_{\text{cl}}$ ;  $-\cdot-\cdot-\cdot$  sum of classical contribution and of first-order quantum correction  $B_{\text{cl}} + \lambda B_{\text{qm},1}$ ;  $-----$  sum of classical contribution as well as of first-order and second-order quantum corrections  $B_{\text{cl}} + \lambda B_{\text{qm},1} + \lambda^2 B_{\text{qm},2}$ ;  $—————$  sum of classical contribution as well as of first-order, second-order and third-order quantum corrections  $B_{\text{cl}} + \lambda B_{\text{qm},1} + \lambda^2 B_{\text{qm},2} + \lambda^3 B_{\text{qm},3}$ .

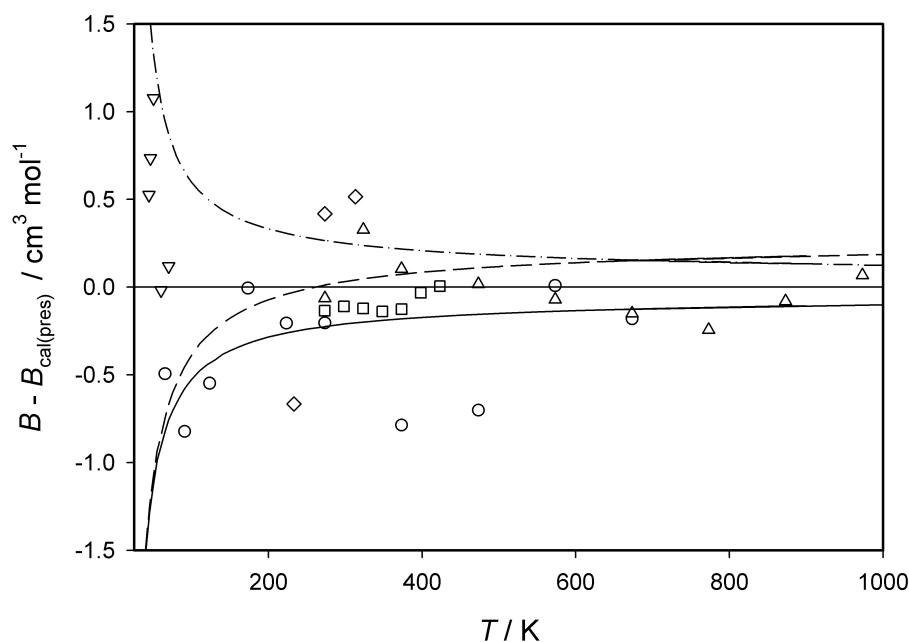


Figure 2. Differences ( $B - B_{\text{cal}(\text{pres})}$ ) of experimental ( $B_{\text{exp}}$ ) and calculated ( $B_{\text{cal}(\text{lit})}$ ) second pressure virial coefficients from values ( $B_{\text{cal}(\text{pres})}$ ) calculated with the new interatomic potential for Ne. Experimental data:  $\circ$  Holborn and Otto [19];  $\Delta$  Nicholson and Schneider [20];  $\square$  Michels et al. [21];  $\nabla$  Gibbons [22];  $\diamond$  Vogl and Hall [23]. Calculated values: — potential by Aziz and Slaman [7]; - · - · potential by Cybulski and Toczylowski [6]; - - - potential by Wüest and Merkt [5].

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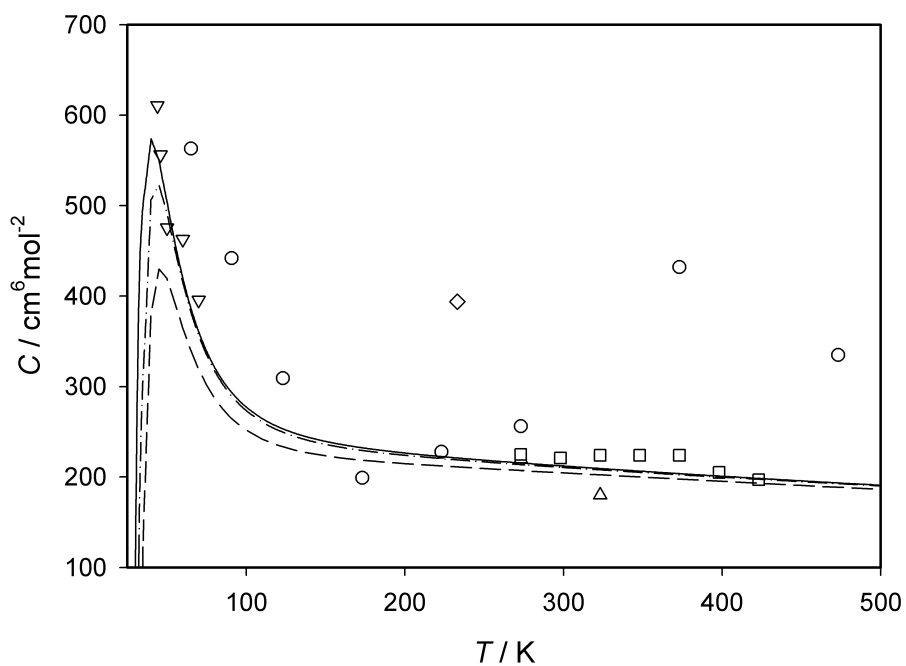


Figure 3. Comparison of experimental data and of calculated values for the third pressure virial coefficient  $C$  derived from the new interatomic potential for Ne. Experimental data:  $\circ$  Holborn and Otto [19];  $\Delta$  Nicholson and Schneider [20];  $\square$  Michels et al. [21];  $\nabla$  Gibbons [22];  $\diamond$  Vogl and Hall [23].

Calculated values: - - - - classical contribution  $C_{\text{add}}$ , - · - · - classical and non-additivity contributions  $C_{\text{add}} + C_{\text{non-add}}$ , ——— sum of classical and non-additivity contributions and of the first-order quantum correction  $C_{\text{add}} + C_{\text{non-add}} + \lambda C_{\text{qm},1}$ .

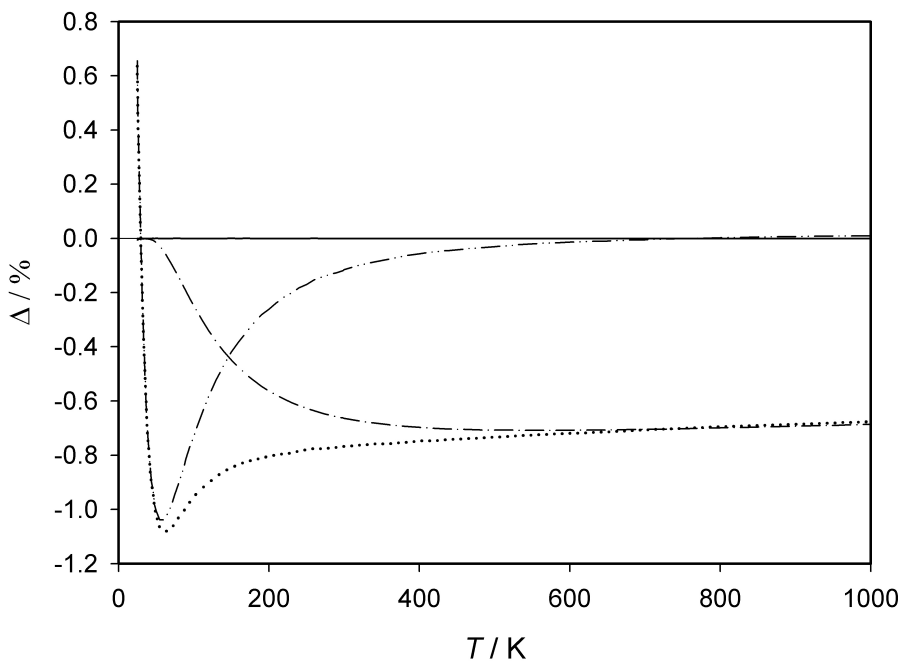


Figure 4. Relative deviations  $\Delta = 100 (\eta - \eta_{qm,5}) / \eta_{qm,5}$  between viscosity values calculated for different approximation procedures and viscosity values resulting from quantum-mechanical calculations up to the fifth-order approximation for the individual  $[\eta_{ij}]_{qm,5}$  within the first-order formulation of  $[\eta_{mix}]_1$  for the new interatomic potential for Ne. Differences related to: ..... first-order classical calculation  $[\eta]_{cl,1}$ ; - · - · - · - · fifth-order classical calculation  $[\eta]_{cl,5}$ ; - - - - - first-order quantum-mechanical calculation  $[\eta_{mix}]_{qm,1}$ .

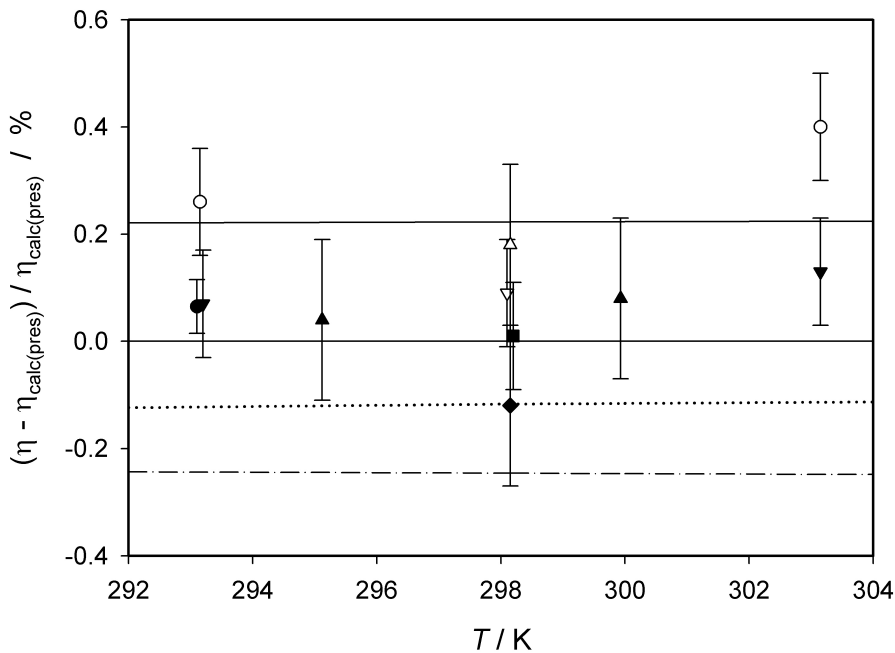


Figure 5. Relative deviations of experimental and calculated viscosity coefficients from values  $\eta_{cal(pres)}$  calculated quantum-mechanically with the new interatomic potential for Ne near to room temperature. Experimental data with uncertainties characterized by error bars: ● Kestin and Leidenfrost [24]; ○ Kestin and Nagashima [25]; ▼ DiPippo et al. [26]; ▽ Kestin et al. [27], best estimate; ■ Flynn et al. [28]; △ Vogel [29], fitted value; ▲ Vogel [29], experimental data corrected according to new helium standard; ◆ Evers et al. [30]. Calculated values: ..... fifth-order classical calculation  $[\eta]_{cl,5}$ ; ——— potential by Aziz and Slaman [7]; - · - · - potential by Cybulski and Toczyłowski [6].

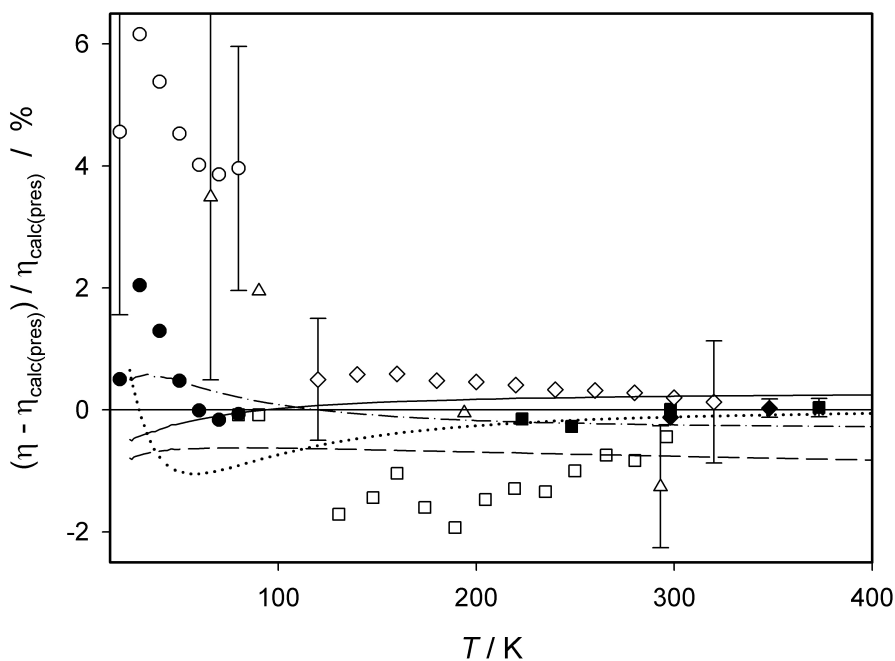


Figure 6. Relative deviations of experimental and calculated viscosity coefficients from values  $\eta_{cal(pres)}$  calculated with the new interatomic potential for Ne at low and medium temperatures. Experimental data with uncertainties characterized by error bars:  $\square$  Johnston and Grilly [32];  $\circ$  Coremans et al. [33];  $\bullet$  Coremans et al. [33], corrected according to new helium standard;  $\Delta$  Rietveld et al. [34];  $\blacksquare$  Flynn et al. [28];  $\diamond$  Clarke and Smith [35];  $\blacklozenge$  Evers et al. [30]. Calculated values:  $\cdots$  fifth-order classical calculation  $[\eta]_{c1,5}$ ;  $\text{—}$  potential by Aziz and Slaman [7];  $-\cdot-\cdot-$  potential by Cybulski and Toczyłowski [6];  $----$  potential by Wüest and Merkt [5].

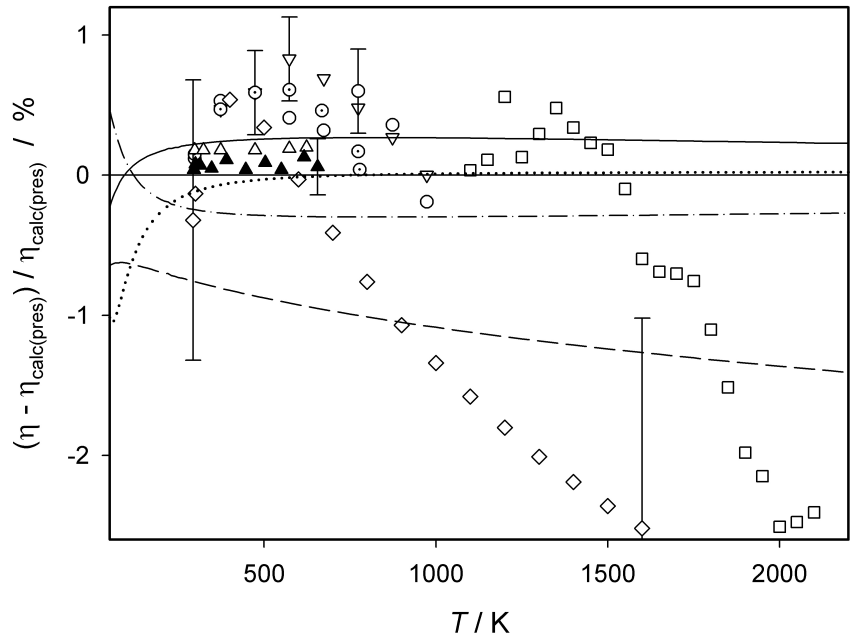


Figure 7. Deviations of experimental and calculated viscosity coefficients from values  $\eta_{\text{cal(pres)}}$  calculated with the new interatomic potential for Ne at higher temperatures. Experimental data with uncertainties characterized by error bars:  $\nabla$  Kestin et al. [27], best estimate;  $\circ$  Hellemans et al. [37];  $\odot$  Kestin et al. [38];  $\diamond$  Dawe and Smith [39];  $\square$  Guevara and Stensland [40];  $\triangle$  Vogel [29], fitted values;  $\blacktriangle$  Vogel [29], experimental data corrected according to new helium standard. Calculated values:  $\cdots$  fifth-order classical calculation  $[\eta]_{\text{cl},5}$ ;  $\text{---}$  potential by Aziz and Slaman [7];  $\text{- - - -}$  potential by Cybulski and Toczyłowski [6];  $\text{---}$  potential by Wüest and Merkt [5].

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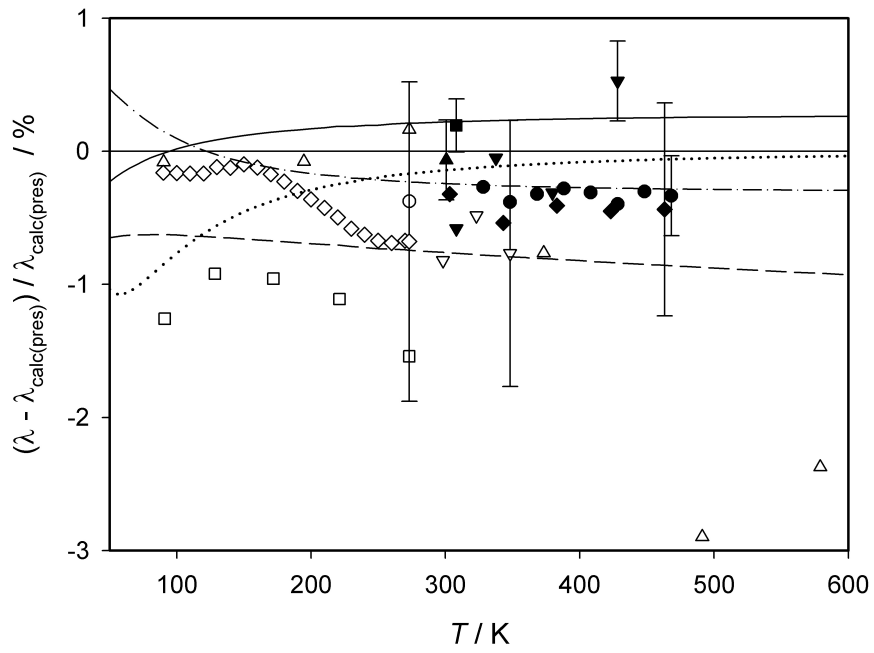


Figure 8. Deviations of experimental and calculated thermal conductivity coefficients from values  $\lambda_{\text{cal(pres)}}$  calculated with the new interatomic potential for Ne at low and medium temperatures. Experimental data with uncertainties characterized by error bars: ● Haarman [43]; ▲ Kestin et al. [44]; ■ Assael et al. [45]; ▼ Millat et al. [46]; ◆ Hemminger [47]; ○ Weber [48]; △ Kannuluik and Carman [49]; □ Keyes [50]; ▽ Sengers et al. [51]; ◇ Nesterov and Sudnik [52], smoothed values. Calculated values: ..... fifth-order classical calculation  $[\eta]_{\text{cl},5}$ ; — potential by Aziz and Slaman [7]; - · - · - · potential by Cybulski and Toczyłowski [6]; - - - - potential by Wüest and Merkt [5].

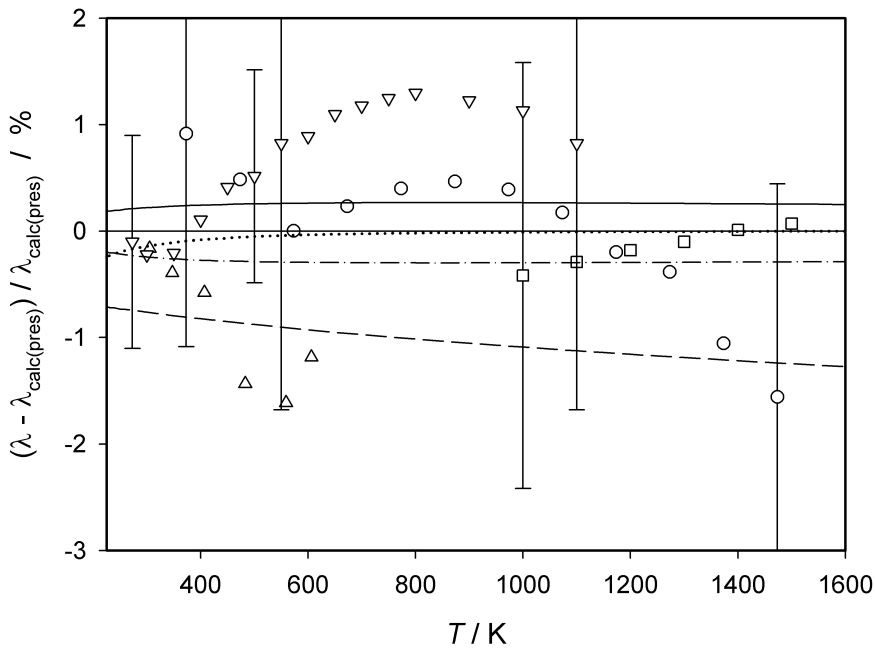


Figure 9. Deviations of experimental and calculated thermal conductivity coefficients from values  $\lambda_{\text{cal(pres)}}$  calculated with the new interatomic potential for Ne at higher temperatures. Experimental data with uncertainties characterized by error bars:  $\circ$  Saxena and Saxena [53], smoothed values;  $\Delta$  Tufeu et al. [54];  $\square$  Springer and Wingeier [55];  $\nabla$  Ziebland [56], recommended values. Calculated values:  $\cdots$  fifth-order classical calculation  $[\eta]_{\text{cl},5}$ ;  $\text{---}$  potential by Aziz and Slaman [7];  $\text{- - - -}$  potential by Cybulski and Toczyłowski [6];  $\text{---}$  potential by Wüest and Merkt [5].

Appendix A: Thermophysical properties of neon calculated in this work

The thermophysical properties of naturally occurring neon are given in table A.

Table A1. Thermophysical properties of neon for the interatomic potential of this work

$T$ (K)	$B$ ( $\text{cm}^3 \text{mol}^{-1}$ )	$C$ ( $\text{cm}^6 \text{mol}^{-2}$ )	$\eta$ ( $\mu\text{Pa}\cdot\text{s}$ )	$\lambda$ ( $\text{mW m}^{-1} \text{K}^{-1}$ )
25.00	-128.50	-1716.	3.9213	6.0597
26.00	-119.87	-1130.	4.0790	6.3033
27.00	-112.02	-689.5	4.2353	6.5446
28.00	-105.04	-358.4	4.3927	6.7878
30.00	-92.972	78.89	4.7097	7.2775
32.00	-82.953	325.4	5.0270	7.7676
34.00	-74.517	461.5	5.3447	8.2585
36.00	-67.316	532.2	5.6617	8.7482
38.00	-61.085	564.7	5.9784	9.2377
40.00	-55.657	574.0	6.2915	9.7214
42.00	-50.888	569.7	6.6035	10.204
44.00	-46.666	557.7	6.9132	10.682
46.00	-42.905	541.5	7.2191	11.155
48.00	-39.526	523.4	7.5245	11.627
50.00	-36.486	504.6	7.8257	12.093
55.00	-30.063	459.3	8.5658	13.237
60.00	-24.892	419.9	9.2862	14.352
65.00	-20.676	387.2	9.9868	15.436
70.00	-17.169	360.6	10.668	16.491
75.00	-14.213	339.9	11.331	17.518
80.00	-11.676	321.5	11.976	18.518
85.00	-9.4909	307.0	12.605	19.493
90.00	-7.5869	295.2	13.217	20.443
95.00	-5.9132	285.4	13.815	21.370
100.00	-4.4329	277.3	14.399	22.277
110.00	-1.9365	264.7	15.528	24.030
120.00	0.0895	255.6	16.612	25.713
130.00	1.7559	248.8	17.654	27.333
140.00	3.1490	243.5	18.660	28.896
150.00	4.3280	239.4	19.634	30.410
160.00	5.3365	236.0	20.579	31.879
170.00	6.2068	233.1	21.498	33.307
180.00	6.9638	230.6	22.394	34.699
190.00	7.6271	228.6	23.268	36.058
200.00	8.2116	226.5	24.122	37.385
210.00	8.7298	224.7	24.958	38.685
220.00	9.1906	223.1	25.778	39.959
230.00	9.6037	221.5	26.583	41.210
240.00	9.9744	220.0	27.372	42.436
250.00	10.308	218.6	28.149	43.643
260.00	10.610	217.3	28.912	44.829
270.00	10.884	215.9	29.665	45.999
273.15	10.964	215.5	29.900	46.364
280.00	11.133	214.6	30.408	47.153
290.00	11.360	213.9	31.139	48.289

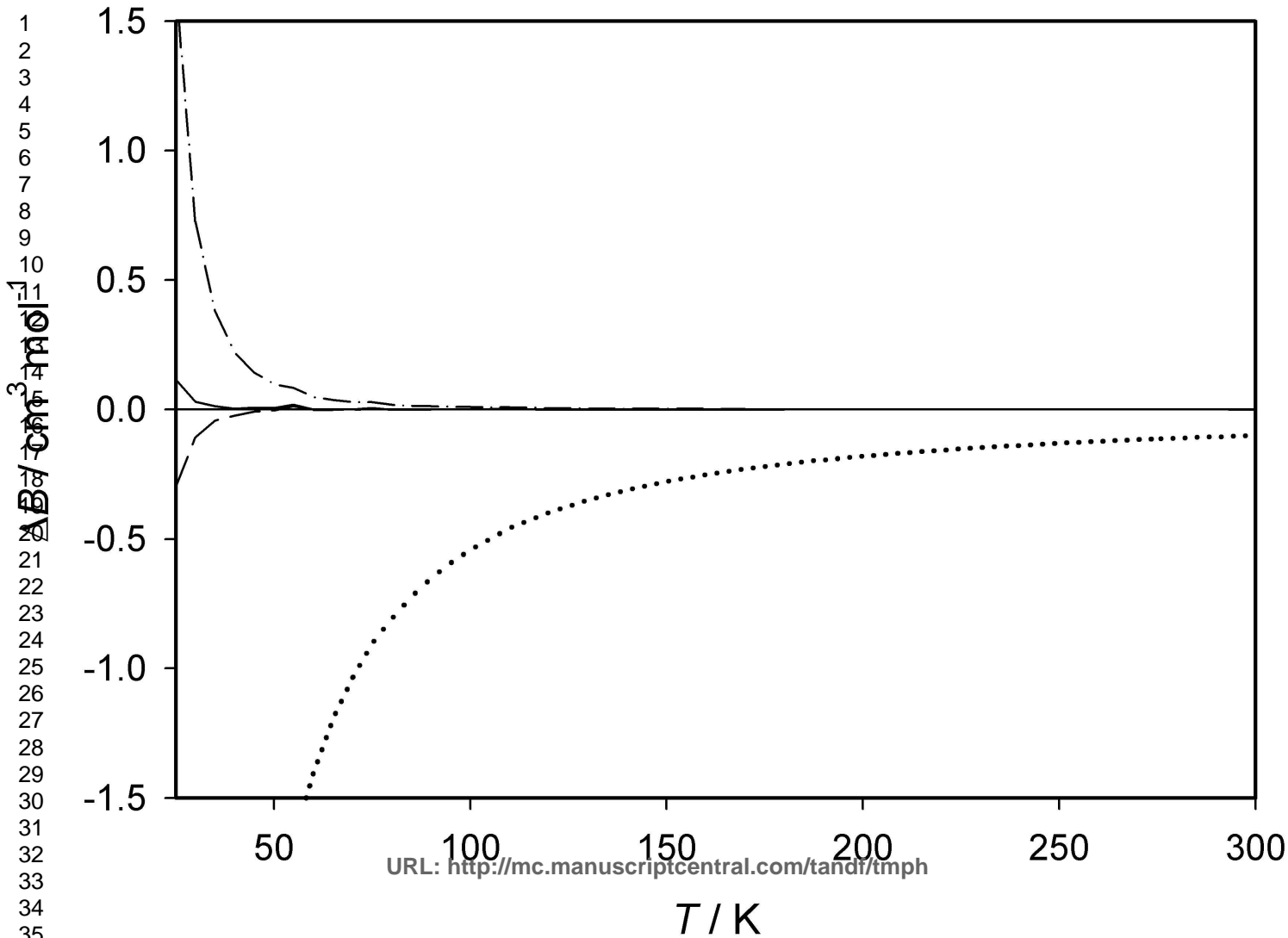
Table A2. Table continued

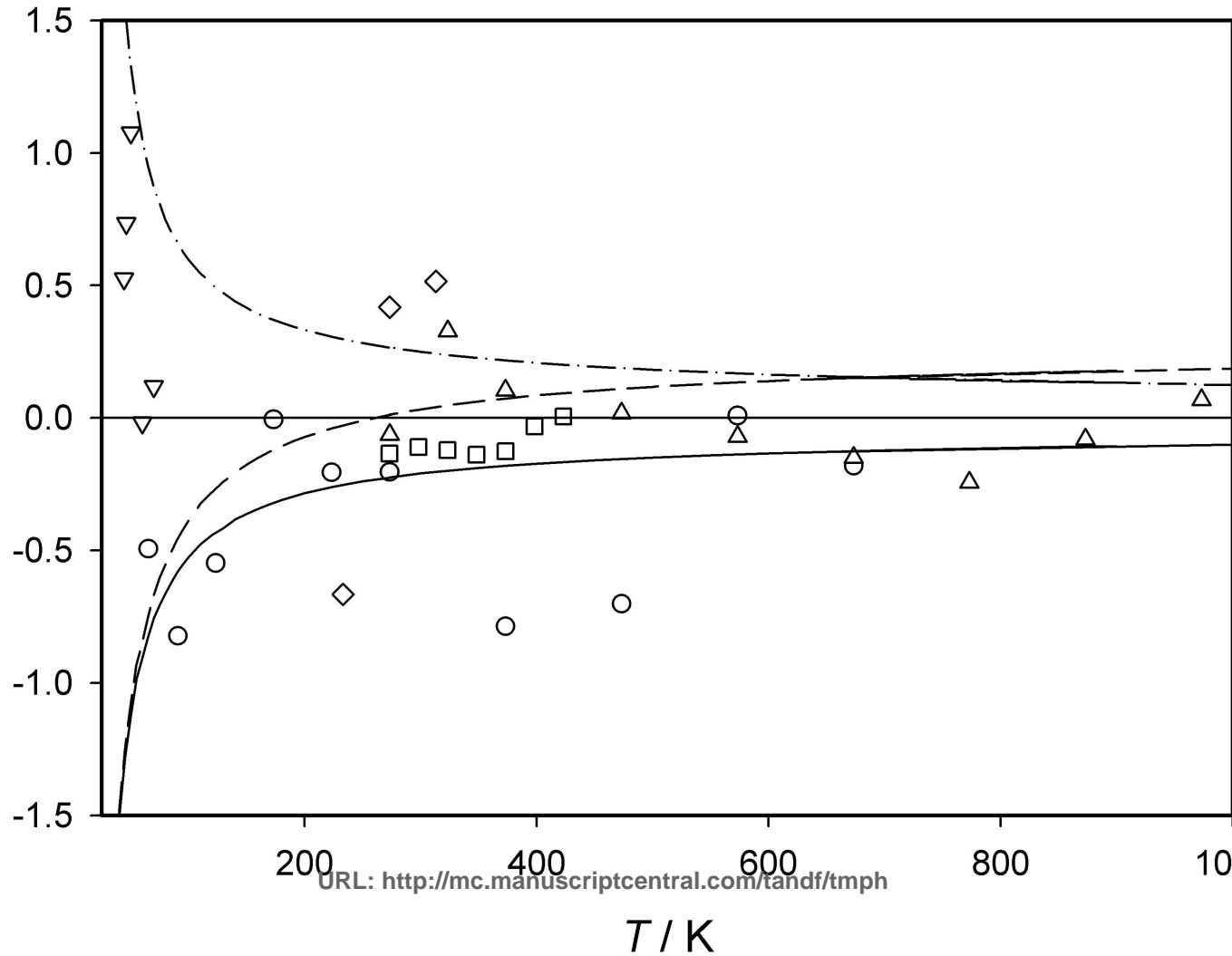
$T$ (K)	$B$ (cm <sup>3</sup> mol <sup>-1</sup> )	$C$ (cm <sup>6</sup> mol <sup>-2</sup> )	$\eta$ ( $\mu$ Pa.s)	$\lambda$ (mW m <sup>-1</sup> K <sup>-1</sup> )
298.15	11.530	212.9	31.728	49.203
300.00	11.567	212.2	31.860	49.410
320.00	11.930	209.8	33.277	51.610
340.00	12.237	207.4	34.660	53.758
360.00	12.497	205.2	36.014	55.859
380.00	12.719	203.0	37.339	57.917
400.00	12.909	200.8	38.640	59.937
420.00	13.072	198.8	39.918	61.921
440.00	13.212	196.7	41.174	63.871
460.00	13.333	194.8	42.411	65.789
480.00	13.437	192.8	43.628	67.679
500.00	13.527	190.9	44.829	69.542
550.00	13.700	186.4	47.761	74.091
600.00	13.819	182.1	50.604	78.502
650.00	13.896	178.0	53.370	82.793
700.00	13.943	174.2	56.068	86.977
750.00	13.968	170.6	58.703	91.065
800.00	13.975	167.2	61.284	95.067
850.00	13.968	163.9	63.814	98.9901
900.00	13.952	160.8	66.298	102.84
950.00	13.927	157.9	68.739	106.63
1000.00	13.895	155.1	71.141	110.35
1100.00	13.819	149.9	75.838	117.63
1200.00	13.730	145.1	80.408	124.72
1300.00	13.634	140.7	84.866	131.63
1400.00	13.534	136.7	89.223	138.38
1500.00	13.432	132.9	93.489	144.99
1600.00	13.329	129.5	97.674	151.48
1700.00	13.226	126.2	101.78	157.85
1800.00	13.125	123.2	105.83	164.11
1900.00	13.025	120.3	109.80	170.28
2000.00	12.926	117.6	113.72	176.35
2100.00	12.830	115.1	117.59	182.34
2200.00	12.736	112.7	121.40	188.25
2300.00	12.644	110.4	125.17	194.08
2400.00	12.554	108.2	128.89	199.85
2500.00	12.467	106.2	132.57	205.55
2600.00	12.381	104.2	136.21	211.19
2700.00	12.298	102.4	139.81	216.76
2800.00	12.216	100.6	143.38	222.29
2900.00	12.137	98.92	146.91	227.76
3000.00	12.059	97.29	150.41	233.18
3100.00	11.984	95.73	153.87	238.55
3200.00	11.910	94.24	157.31	243.88
3300.00	11.838	92.80	160.72	249.16
3400.00	11.767	91.41	164.11	254.40
3500.00	11.698	90.08	167.46	259.60
3600.00	11.631	88.80	170.79	264.76
3700.00	11.565	87.56	174.10	269.88
3800.00	11.501	86.36	177.39	274.97
3900.00	11.438	85.21	180.65	280.02
4000.00	11.376	84.09	183.89	285.04

Table A3. Table continued

$T$ (K)	$B$ (cm <sup>3</sup> mol <sup>-1</sup> )	$C$ (cm <sup>6</sup> mol <sup>-2</sup> )	$\eta$ ( $\mu$ Pa.s)	$\lambda$ (mW m <sup>-1</sup> K <sup>-1</sup> )
4100.00	11.316	83.01	187.11	290.03
4200.00	11.257	81.96	190.31	294.99
4300.00	11.199	80.95	193.49	299.91
4400.00	11.142	79.96	196.65	304.81
4500.00	11.087	79.01	199.80	309.68
4600.00	11.032	78.09	202.92	314.52
4700.00	10.979	77.19	206.03	319.33
4800.00	10.926	76.31	209.12	324.12
4900.00	10.875	75.46	212.20	328.88
5000.00	10.825	74.64	215.26	333.62
6000.00	10.366	67.45	245.09	379.81
7000.00	9.9770	61.77	273.72	424.15
8000.00	9.6396	57.14	301.40	467.00
9000.00	9.3429	53.30	328.28	508.61
10000.00	9.0788	50.05	354.48	549.16

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