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Equilibrium and Transport Properties of Eleven Polyatomic Gases At Low Density

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This study presents a computer programmable, thermodynamically consistent representation of the second virial coefficient B, viscosity η, self-diffusion coefficient D, and isotopic thermal diffusion factor α_0 of the eleven gases: N_2, O_2, NO, CO, N_2O, CO_2, CH_4, CF_4, SF_6, C_2H_4, and C_2H_6, all at low density. Limited thermodynamic consistency is achieved by the use of four scaling parameters (σ, c, V_0^*, ρ^*) in addition to the molecular weight. In terms of these parameters, the collision integrals for the transport properties obey a single law of corresponding states. Furthermore, $\Omega^{(2,2)*}(T)$ is the same as that for the universal correlation of the monatomic gases [J. Phys. Chem. Ref. Data 13, 229 (1984)], whereas $\Omega^{(1,1)*}(T)$ is only slightly modified. The same parameters nearly correlate the spherical part $B_0(T) = B(T) - B_{ns}(T)$ of the second virial coefficient corrected for the most important nonspherical influences; its dimensionless form $B_0^*(T)$ differs from that for the monatomic gases and also, somewhat, for each of the eleven gases, except that one form suffices for N_2, O_2, NO, CO. The correlations embrace the reduced temperature range $1 < T^* < 10$ with the parameters σ and ϵ, and the range $T^* > 10$ with the parameters V_0^* and ρ^* derived from high-energy beam experiments. The accuracy achieved is carefully specified, and the correlation can be used in a predictive mode.

Key words: corresponding states; isotopic thermal diffusion factor; polyatomic gases, equilibrium properties; polyatomic gases, transport properties; second virial coefficient; self-diffusion coefficient; viscosity.

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List of Symbols

A^*	ratio of collision integrals, Eq. (C6)
B	second virial coefficient
B^*	reduced second virial coefficient, Eq. (B3); ratio of collision integrals, Eq. (C7)
B^*_{ns}	reduced nonspherical contribution to B^*, Eq. (B3)
B^*_0	reduced spherical contribution to B^*, Eq. (B3)
C^*	ratio of collision integrals, Eq. (C8)
C_6	long-range dispersion coefficient
C^*_6	low-temperature scaling parameter, Table A4
D	self-diffusion coefficient
E^*	ratio of collision integrals, Eq. (C9)
F^*	ratio of collision integrals, Eq. (C10)
f_{D}	higher-order correction factor for self-diffusion coefficient, Eq. (C4)
f_η	higher-order correction factor for viscosity, Eq. (C2)
k	Boltzmann constant
M	molecular weight
m	mass of a molecule
N_{A}	Avogadro constant
P	pressure
R	universal gas constant
r	molecule separation in pair potential
T	temperature
T^*	reduced temperature, kT/ϵ
V_0	short-range energy parameter, Eq. (1)
V^*_0	high-temperature scaling parameter, Eq. (2a)
α_0	isotopic thermal diffusion factor, Eq. (C5)

ϵ	energy scaling parameter
η	viscosity
κ	polarizability anisotropy, Table A4
κ_0	higher-order correction for thermal diffusion factor, Eq. (C5a)
μ_0	dipole moment
μ^*	reduced dipole moment, Table A4
ρ	short-range length parameter, Eq. (1)
ρ^*	high-temperature scaling parameter, Eq. (2b)
Θ	quadrupole moment
Θ^*	reduced quadrupole moment, Table A4
σ	length scaling parameter
$\Omega^{(l,s)*}$	reduced collision integral

1. Introduction

Powerful computers are becoming continuously more widespread in industry as indispensable tools of design analysis. Much of the analytic work connected with the design or optimization of processes has been taken over by complex computer codes. To be effective, such computer codes must be able to call on broad data bases that now replace the fast-obsolescing thermodynamic tables. To safeguard reliable results for the designer, such data bases must produce accurate and reliable numerical information on a vast variety of pure substances and their mixtures, covering large ranges of conditions and composition. Furthermore, various subroutines fitted into a large code must assure thermodynamic consistency within each subroutine and between different subroutines. To achieve these desirable goals, it is necessary to make maximum use of theoretical principles. To make the programming of subroutines manageable, it is necessary to compress the data banks into analytically expressed algorithms. This paper contains our contribution to this effort for 11 molecular gases at low density.

Our previous contribution[1,2] provided a complete set of principles and numerical data for the construction of a data base encompassing the five noble gases and all of their multicomponent mixtures at low density. This simultaneous correlation of the equilibrium and transport properties of the very simple monatomic gases was successful because it was based on a combination of the extended principle of corresponding states due to Kestin, Ro, and Wakeham,[3] and a knowledge of the interatomic potentials[4] of the 31 binary interactions characteristic of the set. In its final form,[2] the correlation can be used in a predictive mode, because the application of proven theory has assured complete thermodynamic consistency between the different properties of a single system as well as between different systems included in the set. The theory consisted of the use of the Boltzmann equation and its solutions due to Chapman and Enskog, and to subsequent workers.[5-8] Furthermore, it was possible to incorporate the low- and high-temperature asymptotic forms of the transport collision integrals and the integral for the second virial coefficient (the "functionals" of the solutions). Independent values of the long-range London dispersion coefficients C_6 and C_8 were obtained from a combination of quantum theory with dielectric and optical data, and independent values of the parameters describing the repulsive wall of the potential were obtained from a combination of theoretical calculations with measurements of high-energy beam scattering. Agreement with measurements has been secured in that the material constants of the different systems and the adjustable constants in the expressions for the property functionals have been made consistent with a vast, though limited, body of carefully preselected experimental results.

It is natural to attempt to develop a similar synthesis for the more complex polyatomic gases. In taking this next step, we are fully aware of the fact that the previous and the current algorithms concern systems that are not the most important ones industrially, but we follow a more systematic route, limited only by accessible theory, and hope that these data will prove useful, albeit in a restricted field of applications. For the present study we have chosen 11 gases whose force fields are at least axially symmetric; they are

the linear molecules N_2, O_2, NO, CO, N_2O, CO_2,
the near-spherical molecules CH_4, CF_4, SF_6,
and the near-linear molecules C_2H_4, C_2H_6.

The present task is a more difficult one because

(a) asymptotic forms of the property functionals are complex at low temperatures and are not available for use;

(b) the body of experimental data is less extensive;

(c) no wide-ranging principle of corresponding states is available, although a more restricted one will be introduced later;

(d) the kinetic-theory base available is severely restricted and essentially limited to the use of the Monchick–Mason type of conclusions about nonspherical effects on transport properties.[9,10]

It follows from the preceding remarks that the present correlation must be a limited one. First, it will be restricted to the low-density calculation of viscosity η, self-diffusion coefficient D, isotopic thermal diffusion factor α_0, and second virial coefficient B. We recall that a knowledge of the second virial coefficient $B(T)$ combined with that of the ideal-gas specific heat $C_v^\circ(T)$ or $C_p^\circ(T)$ is equivalent to a fundamental equation from which all thermodynamic equilibrium properties at low density can be calculated. Since the specific heats can be calculated from statistical thermodynamics,[11] we refrain from listing formulas for them. Second, the temperature range will be more restricted ($T^* > 1$, where $T^* = kT/\epsilon$ and ϵ is the potential well-depth parameter) owing to the unavailability of low-temperature asymptotic forms of the property functionals. Third, we do not yet include the explicit effects of the internal degrees of freedom on the transport properties, and this rules out the calculation of thermal conductivity. Fourth, the resulting accuracy of prediction is a more modest one. Finally, we leave the treatments of mixtures and of quantum effects to future reports.

2. Methodology

It should be clear from the foregoing discussion that we must concentrate our efforts on taking into account the lack of spherical symmetry of the relevant intermolecular potentials, that is to include or somehow to bypass the effects of anisotropy of the long-range dispersion energy and of the short-range steric repulsion, the effects of permanent molecular dipoles, quadrupoles, and so on. The most significant step to accomplish this end is the omission of reduced temperatures less than $T^* = 1$. There are two immediate reasons for this omission, and three important consequences thereof. The reasons are as follows:

(1) Lack of asymptotic low-temperature forms for property functionals that can be determined independently, so that the range between $T^* = 0$ and $T^* = 1$ can be covered by interpolation rather than by extrapolation. In the case of transport coefficients the cause of this lack is the existence of several long-range contributions to the intermolecular potential whose effects on the low-temperature properties are neither clearly separable nor even individually calculable (owing to the nonsphericity). The most important of these contributions are the r^{-6} dispersion and dipole-induction energies, the r^{-5} quadrupole–quadrupole energy, the r^{-4} dipole–quadrupole energy, and the r^{-3} dipole–dipole energy, all of which are orientation dependent.[12] In the case of second virial coefficients, the cause of the lack is our ignorance about the detailed shape of the intermolecular potential around its minimum, which is the region that controls the low-temperature behavior.

(2) Lack of experimental information at low temperatures that could be used to compensate for the above theoretical ignorance.

The important useful consequences of restricting the correlation to $T^* > 1$ are as follows:

(1) The transport coefficients are determined by only the repulsive branch of the intermolecular potential.[13] This branch is monotonic and rather featureless, so that a limited two-parameter principle of corresponding states can be formulated. That is, an effective average spherical potential can be represented by two scaling parameters σ and ϵ, which can be determined from viscosity data. Even though this repulsive branch depends on molecular orientation, the effect of this orientation dependence on the transport coefficients is indicated to be weak by model calculations.[9,10] Moreover, the resulting corresponding-states property functionals should be virtually the same as for the noble gases, except for the strongest polar gases.[13]

(2) The effects of the orientation dependence of the potential on the second virial coefficients, although not negligible, can be calculated with the aid of existing theory, which gives the form of a high-temperature series expansion. Derivations and tabulations of auxiliary functions for this purpose have been given in a companion paper.[14]

(3) The average effective repulsive wall of the potential, as found from application of a limited principle of corresponding states to viscosity data, can be extended to encompass higher temperatures with the help of data on the scattering of high-energy atomic and molecular beams. This allows us to make an extension of the property functionals to high temperatures with the same extended corresponding-state correlation as used for the noble gases.

3. Limited Principle of Corresponding States

The central idea that emerges from the foregoing methodology is thus to use viscosity data to determine the parameters for a limited principle of corresponding states that is related to an effective spherical intermolecular potential. The resulting spherical-potential correlation can then be used to calculate self-diffusion coefficients and isotopic thermal diffusion factors, as well as a spherical contribution to the second virial coefficients $B_0(T)$. To the latter must be added nonspherical contributions $B_{\rm ns}(T)$, which can be calculated from known molecular parameters such as quadrupole moments and polarizability anisotropies. As will be demonstrated, this procedure works well for the transport coefficients, although not quite to the level of accuracy achieved with the noble gases, but less well for the second virial coefficients. In particular, the reduced function for $B_0(T)$ is not quite the same for all the molecular gases considered; this is not too surprising, because the procedure we use concentrates all possible discrepancies, from whatever source, in this functional.

The specific procedure is to utilize the same principle of corresponding states for the transport coefficients of molecular gases as was used for the noble gases in the middle temperature range,

$$1 < T^* < 10.$$

The same types of property functionals are used, and the same types of scaling parameters σ and ϵ. The material parameter C_6^* that appeared in the improved corresponding-states principle for the noble gases is not needed here, because we are omitting the cryogenic range ($T^* < 1$). The parameters σ and ϵ are determined from experimental viscosity data, using the same viscosity functional $\Omega^{(2,2)*}$ that was used for the noble gases. In the case of the noble gases the functional $\Omega^{(2,2)*}$ uniquely determined the functional $\Omega^{(1,1)*}$ for D and α_0 through an inversion procedure for the interatomic potential.[1,2,13] This inversion is not strictly possible in the case of the present molecular gases because we are dealing with only an effective spherical potential. The functional $\Omega^{(1,1)*}$ for the noble gases is thus not necessarily expected to be suitable for molecular gases, although calculations with model anisotropic potentials[9,10] indicate that it should be a good approximation. In practice, only small deviations from accurate experimental results were found. A small adjustment was therefore applied to the noble-gas functional $\Omega^{(1,1)*}$ to produce improved agreement; the adjustment leaves $\Omega^{(1,1)*}$ unchanged at $T^* = 10$ and about 3% smaller at $T^* = 3$. The functionals for other collision integrals needed to calculate D and α_0 (see Appendix C for formulas) make only small contributions to the final results and were therefore not adjusted. Thus the parameters σ and ϵ, determined from η, directly predict D and α_0 with no explicit corrections for the effects of the nonsphericity of the potential.

The parameters σ and ϵ are also used to calculate an effective spherical contribution to the second virial coefficient. The corresponding reduced functional, $B_0^*(T^*)$, has the same form as for the noble gases, but the numerical values of its coefficients differ, and indeed vary somewhat among the different molecular gases. The functionals $B_0^*(T^*)$ were constructed by first calculating the nonspherical contributions to the second virial coefficient

$B_{ns}(T)$ by means of the method and tabulations of auxiliary functions given in Ref. 14. This method is based on an existing theory in which anisotropic contributions are added to an effective spherical potential, and the nonspherical contributions $B_{ns}(T)$ calculated as a high-temperature series expansion; the parameters needed for this calculation are given in Appendix A. The results are insensitive to the specific form of the effective spherical potential, but depend on its scaling parameters σ and ϵ.[14] By subtraction of calculated $B_{ns}(T)$ from experimental $B(T)$, and reduction with σ and ϵ, the functionals $B_0^*(T^*)$ were obtained. They were not quite universal, but were somewhat different for each new molecular gas considered, nor were we able to achieve universality by adjustment of σ, ϵ, and the viscosity functional $\Omega^{(2,2)*}$. This is depicted in Fig.1, which illustrates the fact that one functional covers the four gases: N_2, O_2, NO, and CO, which is different from those for CH_4, CF_4, and SF_6. The curves for the remaining four gases of this set (N_2O, CO_2, C_2H_4, and C_2H_6) are shown in Fig. 2. Notice that all the curves join together at $T^* = 10$. It is somewhat disappointing that one functional $B_0^*(T^*)$ does not suffice for all gases, but it is not especially surprising in view of the fact that the theoretical treatment of the effects of nonspherical potentials on both transport properties and second virial coefficients is still in a rudimentary state.

In the high-temperature range,

$$T^* > 10,$$

all the properties are dominated by an effective spherical repulsive potential, which can be represented by the form,

$$V(r) = V_0 \exp(-r/\rho), \tag{1}$$

where V_0 and ρ are parameters deduced from high-energy beam scattering experiments. Two additional dimensionless material parameters are thereby introduced into the correlation,

$$V_0^* = V_0/\epsilon, \tag{2a}$$

$$\rho^* = \rho/\sigma. \tag{2b}$$

These parameters are used in the same high-temperature functionals as those for the noble gases. The functionals from the middle temperature range are joined smoothly (continuous through second derivatives) to these high-temperature functionals at $T^* = 10$. The effect of different values of V_0^* and ρ^* on the functional $B_0^*(T^*)$ can be seen in Fig. 1.

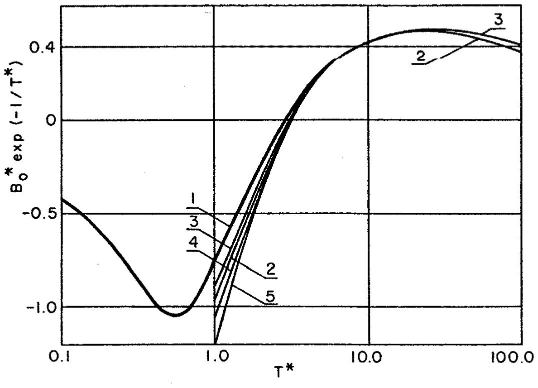

FIG. 1. Correlation of spherical, reduced second virial coefficient, B_0^*, as a function of reduced temperature. (1) Najafi *et al.*[2]; (2) N_2, O_2, NO, CO; (3) CH_4; (4) CF_4; (5) SF_6.

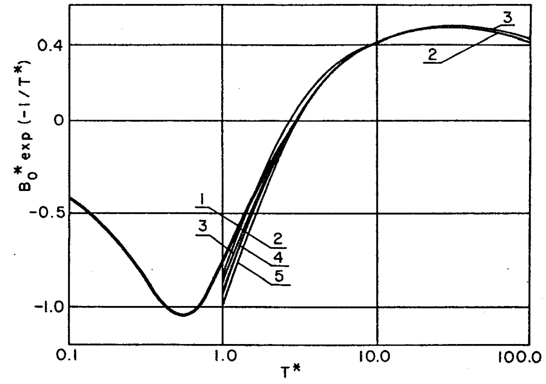

FIG. 2. Correlation of spherical, reduced second virial coefficient, B_0^*, as a function of reduced temperature. (1) Najafi *et al.*[2], (2) CO_2; (3) N_2O; (4) C_2H_4; (5) C_2H_6.

In summary, the correlation of the transport coefficients η, D, and α_0, and of the spherical contributions to the second virial coefficients B_0, requires only the scaling parameters σ, ϵ, V_0^*, and ρ^*, in addition to the molecular weights. Other parameters are needed only for the calculation of the nonspherical contributions to the second virial coefficients.

It is important to stress that the present correlation can still operate in a predictive mode, in spite of the fact that the functional $B_0^*(T^*)$ is not universal, and that the accuracy is somewhat less than for the noble gases. The three main types of prediction are as follows:

(1) The viscosity is predicted over a much wider temperature range than that for which direct measurements exist, including the high-temperature range made accessible by beam measurements. Only limited viscosity data are needed to fix the values of the parameters σ and ϵ.

(2) The transport coefficients D and α_0 are predicted over a similar wide temperature range on the basis of limited viscosity measurements. No direct measurements of either D or α_0 are required.

(3) Second virial coefficients are predicted over a much wider range than that for which direct measurements exist, including the high-temperature range. Only limited data on $B(T)$ are needed to determine which reduced $B_0^*(T^*)$ curve should be used.

4. Parameters and Functionals

Parameters are given in Appendix A, the functionals $\Omega^{(2,2)*}$, $\Omega^{(1,1)*}$, and B_0^* in Appendix B, and the general formulas for their use in Appendix C.

Table A1 contains values of the universal physical constants employed in this work,[15] and Table A2 lists the values of the molecular weights of the gases.[16] Table A3 lists the values chosen for the four scaling parameters σ, ϵ/k, ρ^*, and V_0^*.

The parameters σ and ϵ/k were determined, as already mentioned, by fitting accurate viscosity data to the same functional $\Omega^{(2,2)*}$ as used for the noble gases,[1,2] in the range $1 \leqslant T^* \leqslant 10$. The values in Table A3 are nearly the same as earlier values reported by the original experiments.[17–20] Slight real differences exist because we have used a somewhat different expression for $\Omega^{(2,2)*}$ than did the earlier workers. A general large difference, which is only apparent and not real, occurs because different normalization constants have been used. (Only relative values of σ and ϵ have physical significance.) The values in Table A3 have been normalized with respect to argon, for which we assume

$$\sigma = 0.3350\ \text{nm}, \quad \epsilon/k = 141.5\ \text{K},$$

corresponding to a realistic Ar–Ar potential reported by Aziz and Chen.[21]

The parameters ρ and V_0 were obtained indirectly by calculation from the results of various scattering measurements that probe the repulsive wall of the potential. The results of these atom–atom, atom–molecule, and molecule–molecule measurements can be decomposed into effective atom–atom potentials between atoms in different molecules, from which various other molecule–molecule potentials can be built up.[22,23] We have used the N$\cdots$N, O$\cdots$O, and N$\cdots$O effective potentials summarized by Cubley and Mason[24] to generate effective molecule–molecule potentials for N_2, O_2, NO, and N_2O, which were then fitted by the exponential form of Eq. (1). The CO potential was taken to be the same as the N_2 potential, since direct scattering measurements[23] with Ar beams show N_2 and CO to be virtually identical in this region. The CO_2 potential was built up by assuming the central C atom to behave like an N atom; the results are insensitive to this assumption because the central atom in a linear triatomic molecule contributes very little to the overall effective molecule–molecule potential.[25] The CH_4 potential was obtained via a combination rule from measurements on the Ar–CH_4 system[26] and on the Ar–Ar system.[24] The CF_4 and SF_6 potentials were similarly obtained from measurements on the He–CF_4 system[27] and the He–SF_6 system.[28] No measurements were available from which reliable estimates of the short-range repulsive potentials for C_2H_4 and C_2H_6 could be obtained and thus the present correlation does not extend above $T^* = 10$ for these gases.

Table A4 lists the material parameters needed for the calculation of the nonspherical contributions to the second virial coefficients.

5. Experimental Data

The experimental data considered in this work were contained in about 2500 references. These were based on one computer output supplied to us by the Purdue University Center for Information and Numerical Data Analysis and Synthesis (CINDAS) and another, provided by Project MIDAS[29] of the University of Stuttgart operated under the direction of Professor K. Stephan with the cooperation of Dr. A. Laesecke. Both computer outputs were supplemented with citations from our own resources. All references were scrutinized and reduced to 147 on which our correlations were ultimately based. The latter were read, critically evaluated, and divided into two classes called primary data (PD) and secondary data (SD).

The division into two classes was based on several objective and subjective criteria. These were: (a) a subjective assessment of the reliability of the data, guided by an examination of internal consistency of error analysis and reproducibility; (b) the authors' statement of precision and accuracy; (c) a direct intercomparison of results from different laboratories and of results obtained by different methods; and (d) an evaluation of the capability of the method used and of the theory of the instrument.

The primary data were exclusively used in the correlation codes to determine optimum functional forms and parameters. Secondary data served to assess the validity of the gross behavior determined by the codes. The references listed in the bibliography of Appendix E refer to both classes of papers, PD as well as SD.

6. Validation, Deviation Plots, and Accuracy

In contrast with Ref. 2, the available experimental data of very high quality could not be subdivided into a set for correlation and a set for validation. For this reason, as already stated, validation with respect to secondary data could not be made very demanding. Appendix D contains 40 deviation plots (Figs. 4–43). In cases where the volume of data allowed it, we prepared separate deviation plots for PD and SD. In such cases, the first plot illustrates the quality of the optimization scheme, and the second gives a gross idea about its general validity. In other cases, there were so few data that we composed them into a single deviation plot to serve both purposes.

In a number of cases the deviations appear to be systematic. It is important to note that this does not prevent the present correlation from operating in a predictive mode, especially in the form of extensions to higher temperatures, because of the utilization of the beam data and the theoretical requirement that the functionals merge at $T^* = 10$.

The deviation plots have been used as a basis of an estimate of accuracy. In most cases, this was determined by the

TABLE a. Estimates of accuracy in the temperature range indicated

System	Temperature range K	B (10^{-3} m^3/kmol)	η %	D %
N_2	100–1300	2.2	0.8	1.0
O_2	130–1400	1.6	0.6	(4.0)[a]
NO	150–1300	(3.5)[a]	1.0	(5)[b]
CO	150–600	2.3	0.8	2.0
N_2O	270–800	2.5	0.8	(5)[b]
CO_2	250–1500	2.5	0.9	(5.0)[a]
CH_4	150–650	1.0	0.6	2.0
CF_4	200–900	2.7	0.3	(5)[b]
SF_6	210–1200	6.0	0.5	(5)[b]
C_2H_4	250–500	1.0	0.5	(4.0)[a]
C_2H_6	250–500	1.0	0.5	(4.0)[a]

[a] Estimate based on secondary data alone.
[b] Estimate made by analogy in the absence of data in the open literature.

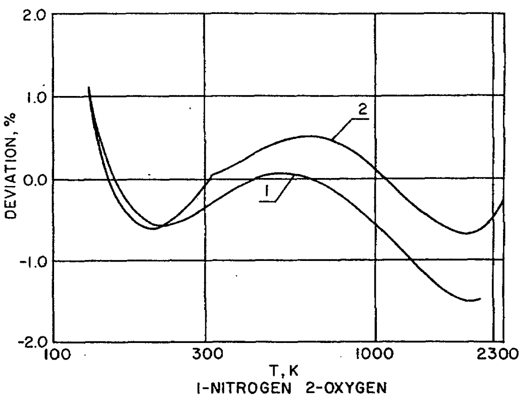

FIG. 3. Deviation of Imperial College (IC) correlation due to Cole and Wakeham (Ref. 30) from Brown (B) correlation.

maximum deviation of 70% of the experimental points in the diagram which are closest to the correlation. In some cases the paucity or even absence of experimental data forced us to make subjective estimates by analogy.

The results of these interpretations are summarized in Table a. Estimates based on secondary data alone are distinguished by a superscript a, and those arrived at by analogy are marked by a superscript b.

7. Comparison with Calculations from Imperial College

Cole and Wakeham of Imperial College[30] correlated the experimental data on the viscosity of nitrogen and oxygen, but limited the use of a principle of corresponding states to temperatures above 316 K. This enabled them to cover a wider range of temperatures in each case (110–2100 K for N_2 and 110–2500 K for O_2) and to achieve a generally smaller uncertainty of fit. However, the price paid for these two advantages consists in the fact that the possibility of employing the correlation in a predictive mode below 316 K has been lost; only interpolation can be made with assurance. The two analyses can thus be looked upon as complementing each other.

The diagram of Fig. 3 plots the deviation of the correlation of Cole and Wakeham[30] from that in the present paper.[d)] The maximum difference is one of 1.0% for N_2 and 0.5% for O_2. On the whole, the two correlations can be said to agree very closely, except at the lowest temperatures where the correlation of Ref. 30 takes over from ours.

Rather similar remarks apply to a more recent correlation of the viscosities of CO_2, CH_4, and SF_6 by Maitland, Trengove, and Wakeham,[31] who made no use of a principle of corresponding states. They achieved a better fit and were able to go to somewhat lower temperatures ($T^* < 1$), but thereby gave up the use of the correlation in a predictive mode, so that the two analyses are again complementary.

8. Description of the Tables

The tables of numerical data are not meant to be exhaustive and have not been designed for linear interpolation. They are convenient extracts only, because the algorithm for each property can be programmed on a computer on the basis of the information supplied here. A more extensive tabulation would be prohibitive in its volume.

The eleven tables, one for each gas, are identical in their structure and indicate values of B, η, D, and α_0 in SI units. Below 0 °C, the temperatures are listed in kelvins, above that in degrees Celsius in conformity with the common practice prevailing at this time.

[d)] Reference 30 contains a typographical error. The matching temperature for the two equations on p. 216 which represent the viscosity of oxygen should read $T^* = 2.5$ or $T = 316$ K (communicated to authors by W. A. Wakeham).

9. Tables

TABLE 1. Properties of nitrogen as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
100 K	− 160.94	6.73	0.0280	− 0.0037
150	− 72.19	10.06	0.0615	0.1981
200	− 35.59	12.99	0.1045	0.3119
250	− 15.44	15.62	0.1558	0.3836
300	− 2.78	18.02	0.2146	0.4317
0 °C	− 8.92	16.75	0.1821	0.4081
20	− 4.22	17.70	0.2061	0.4261
40	− 0.22	18.62	0.2312	0.4417
60	3.22	19.51	0.2573	0.4552
80	6.20	20.38	0.2845	0.4670
100	8.78	21.23	0.3128	0.4774
150	13.92	23.26	0.3878	0.4980
200	17.65	25.18	0.4688	0.5131
250	20.38	27.01	0.5557	0.5242
300	22.41	28.77	0.6482	0.5323
350	23.92	30.47	0.7461	0.5381
400	25.05	32.10	0.8494	0.5423
450	25.91	33.69	0.9579	0.5451
500	26.57	35.23	1.0715	0.5469
600	27.53	38.20	1.3137	0.5483
700	28.27	41.04	1.5753	0.5476
800	29.20	43.77	1.8558	0.5456
900	29.80	46.41	2.1547	0.5403
1000	30.31	48.99	2.4722	0.5325
1500	31.53	61.29	4.3336	0.4856
2000	31.52	72.92	6.6415	0.4486
2500	31.03	84.10	9.3802	0.4221
3000	30.38	94.94	12.5363	0.4023

TABLE 2. Properties of oxygen as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
150 K	− 88.68	11.23	0.0608	0.1009
200	− 48.75	14.75	0.1049	0.2322
250	− 27.38	17.93	0.1578	0.3173
300	− 14.01	20.85	0.2187	0.3762
0 °C	− 20.49	19.31	0.1851	0.3471
20	− 15.54	20.46	0.2099	0.3692
40	− 11.30	21.58	0.2360	0.3886
60	− 7.63	22.66	0.2632	0.4057
80	− 4.44	23.72	0.2914	0.4208
100	− 1.64	24.75	0.3208	0.4342
150	4.02	27.22	0.3989	0.4617
200	8.26	29.55	0.4832	0.4826
250	11.49	31.78	0.5737	0.4987
300	13.98	33.92	0.6699	0.5112
350	15.91	35.97	0.7719	0.5208
400	17.42	37.95	0.8793	0.5284
450	18.61	39.87	0.9922	0.5342
500	19.55	41.73	1.1103	0.5386
600	20.88	45.31	1.3618	0.5444
700	21.75	48.72	1.6333	0.5473
800	22.35	51.99	1.9241	0.5482
900	22.85	55.15	2.2337	0.5478
1000	23.47	58.20	2.5615	0.5488
1500	25.09	72.38	4.4897	0.4761
2000	25.65	85.38	6.8845	0.4530
2500	25.68	97.58	9.6979	0.4519
3000	25.47	109.17	12.8969	0.4551

TABLE 3. Properties of nitric oxide as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
150 K	− 104.85	10.30	0.0595	0.0850
200	− 58.03	13.56	0.1030	0.2189
250	− 33.42	16.52	0.1552	0.3061
300	− 18.18	19.23	0.2153	0.3666
0 °C	− 25.56	17.80	0.1821	0.3367
20	− 19.92	18.87	0.2066	0.3595
40	− 15.09	19.91	0.2323	0.3795
60	− 10.93	20.92	0.2592	0.3971
80	− 7.31	21.90	0.2871	0.4127
100	− 4.13	22.86	0.3162	0.4266
150	2.29	25.15	0.3933	0.4552
200	7.10	27.33	0.4766	0.4770
250	10.78	29.40	0.5660	0.4939
300	13.63	31.39	0.6611	0.5071
350	15.85	33.30	0.7618	0.5174
400	17.60	35.14	0.8680	0.5254
450	18.99	36.92	0.9795	0.5317
500	20.09	38.65	1.0962	0.5366
600	21.66	41.98	1.3447	0.5432
700	22.68	45.14	1.6129	0.5467
800	23.39	48.18	1.9001	0.5481
900	23.94	51.11	2.2059	0.5481
1000	24.72	53.94	2.5297	0.5504
1500	26.44	67.14	4.4407	0.4462
2000	27.00	79.39	6.8551	0.3965
2500	26.96	91.05	9.7271	0.3855
3000	26.65	102.26	13.0222	0.3845

TABLE 4. Properties of carbon monoxide as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
100 K	− 193.69	6.73	0.0280	− 0.0037
150	− 85.02	10.06	0.0615	0.1981
200	− 42.61	12.99	0.1045	0.3119
250	− 19.98	15.62	0.1558	0.3836
300	− 5.99	18.02	0.2146	0.4317
0 °C	− 12.75	16.75	0.1821	0.4081
20	− 7.57	17.70	0.2061	0.4261
40	− 3.18	18.62	0.2312	0.4417
60	0.59	19.51	0.2573	0.4552
80	3.83	20.38	0.2845	0.4670
100	6.64	21.23	0.3128	0.4774
150	12.21	23.26	0.3878	0.4980
200	16.24	25.18	0.4688	0.5131
250	19.20	27.01	0.5557	0.5242
300	21.40	28.77	0.6482	0.5323
350	23.04	30.47	0.7461	0.5381
400	24.27	32.10	0.8494	0.5423
450	25.22	33.69	0.9579	0.5451
500	25.95	35.23	1.0715	0.5469
600	27.02	38.20	1.3137	0.5483
700	27.84	41.04	1.5753	0.5476
800	29.20	43.77	1.8558	0.5456
900	29.80	46.41	2.1547	0.5403
1000	30.31	48.99	2.4722	0.5325
1500	31.53	61.29	4.3336	0.4856
2000	31.52	72.92	6.6415	0.4486
2500	31.03	84.10	9.3802	0.4221
3000	30.38	94.94	12.5363	0.4023

TABLE 5. Properties of nitrous oxide as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
300 K	−127.19	15.01	0.1188	0.0513
0 °C	−153.69	13.62	0.0986	0.0004
20	−133.28	14.66	0.1135	0.0390
40	−116.55	15.68	0.1292	0.0736
60	−102.60	16.68	0.1457	0.1049
80	−90.78	17.66	0.1631	0.1334
100	−80.64	18.62	0.1811	0.1593
150	−60.64	20.95	0.2296	0.2152
200	−45.85	23.16	0.2824	0.2610
250	−34.46	25.28	0.3394	0.2990
300	−25.44	27.32	0.4003	0.3310
350	−18.10	29.28	0.4649	0.3582
400	−12.03	31.18	0.5332	0.3815
450	−6.94	33.01	0.6051	0.4017
500	−2.62	34.78	0.6803	0.4192
600	4.29	38.18	0.8406	0.4479
700	9.50	41.41	1.0136	0.4701
800	13.51	44.49	1.1986	0.4875
900	16.65	47.44	1.3953	0.5013
1000	19.12	50.28	1.6033	0.5122
1500	25.79	63.20	2.8033	0.5408
2000	28.26	74.65	4.2517	0.5481
2500	30.04	85.13	5.9318	0.5448
3000	31.24	94.92	7.8267	0.5600

TABLE 6. Properties of carbon dioxide as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
250 K	−182.06	12.54	0.0831	−0.0021
300	−120.57	15.13	0.1191	0.0946
0 °C	−149.22	13.76	0.0991	0.0461
20	−127.12	14.78	0.1139	0.0829
40	−109.19	15.78	0.1294	0.1158
60	−94.38	16.76	0.1458	0.1456
80	−81.97	17.72	0.1629	0.1726
100	−71.42	18.66	0.1807	0.1972
150	−50.92	20.92	0.2284	0.2500
200	−36.11	23.07	0.2803	0.2930
250	−24.99	25.13	0.3362	0.3285
300	−16.34	27.11	0.3959	0.3583
350	−9.44	29.02	0.4593	0.3835
400	−3.84	30.85	0.5262	0.4050
450	0.77	32.63	0.5965	0.4235
500	4.62	34.35	0.6702	0.4395
600	10.63	37.64	0.8271	0.4654
700	15.02	40.77	0.9962	0.4852
800	18.31	43.75	1.1772	0.5006
900	20.82	46.61	1.3695	0.5125
1000	22.76	49.36	1.5730	0.5217
1500	27.91	61.91	2.7468	0.5445
2000	30.10	73.05	4.1648	0.5482
2500	32.32	83.27	5.8107	0.5473
3000	33.52	92.84	7.6653	0.5566

TABLE 7. Properties of methane as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
200 K	−105.42	7.70	0.1108	0.1011
250	−66.62	9.53	0.1695	0.2051
300	−43.02	11.23	0.2376	0.2791
0 °C	−54.43	10.33	0.1999	0.2422
20	−45.70	11.00	0.2278	0.2703
40	−38.26	11.65	0.2569	0.2951
60	−31.84	12.28	0.2875	0.3173
80	−26.23	12.90	0.3193	0.3371
100	−21.30	13.50	0.3524	0.3550
150	−11.25	14.95	0.4405	0.3925
200	−3.56	16.32	0.5358	0.4221
250	2.46	17.63	0.6381	0.4458
300	7.27	18.88	0.7471	0.4649
350	11.15	20.08	0.8625	0.4806
400	14.33	21.24	0.9842	0.4934
450	16.93	22.36	1.1119	0.5039
500	19.09	23.44	1.2456	0.5127
600	22.37	25.53	1.5302	0.5259
700	24.65	27.50	1.8370	0.5349
800	26.25	29.40	2.1654	0.5409
900	27.39	31.22	2.5146	0.5447
1000	28.22	32.98	2.8842	0.5470
1500	30.89	41.06	5.0233	0.5437
2000	32.52	48.33	7.6393	0.5052
2500	33.33	55.10	10.7150	0.4899
3000	33.63	61.49	14.2128	0.4875

TABLE 8. Properties of carbon tetrafluoride as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
200 K	−218.30	12.09	0.0317	0.1164
250	−137.57	14.93	0.0483	0.2183
300	−88.78	17.56	0.0677	0.2907
0 °C	−112.31	16.17	0.0570	0.2546
20	−94.30	17.21	0.0649	0.2820
40	−78.98	18.22	0.0732	0.3063
60	−65.80	19.20	0.0818	0.3279
80	−54.33	20.16	0.0908	0.3472
100	−44.28	21.09	0.1002	0.3646
150	−23.87	23.33	0.1252	0.4010
200	−8.40	25.46	0.1522	0.4297
250	3.64	27.48	0.1812	0.4525
300	13.16	29.42	0.2121	0.4709
350	20.80	31.28	0.2448	0.4859
400	26.99	33.07	0.2792	0.4981
450	32.03	34.81	0.3154	0.5081
500	36.16	36.49	0.3533	0.5163
600	42.37	39.72	0.4339	0.5287
700	46.61	42.78	0.5208	0.5370
800	49.53	45.72	0.6139	0.5424
900	51.58	48.54	0.7129	0.5457
1000	53.06	51.27	0.8176	0.5475
1500	57.82	63.81	1.4240	0.5406
2000	61.12	74.96	2.1633	0.5277
2500	63.08	85.01	3.0197	0.5471
3000	64.21	94.20	3.9765	0.5741

TABLE 9. Properties of sulfur hexafluoride as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
250 K	− 411.25	12.85	0.0254	0.0865
300	− 276.74	15.34	0.0361	0.1741
0 °C	− 340.38	14.02	0.0302	0.1303
20	− 291.46	15.01	0.0345	0.1635
40	− 250.91	15.97	0.0391	0.1933
60	− 216.79	16.91	0.0439	0.2200
80	− 187.71	17.83	0.0490	0.2441
100	− 162.64	18.72	0.0542	0.2660
150	− 112.98	20.88	0.0682	0.3127
200	− 76.30	22.92	0.0833	0.3503
250	− 48.25	24.88	0.0997	0.3810
300	− 26.25	26.75	0.1170	0.4065
350	− 8.66	28.55	0.1355	0.4278
400	5.64	30.29	0.1549	0.4458
450	17.39	31.96	0.1754	0.4610
500	27.15	33.59	0.1967	0.4740
600	42.18	36.70	0.2423	0.4946
700	52.94	39.66	0.2913	0.5099
800	60.77	42.48	0.3438	0.5213
900	66.54	45.19	0.3996	0.5297
1000	70.83	47.80	0.4587	0.5360
1500	81.22	59.72	0.7996	0.5481
2000	86.66	70.37	1.2122	0.5453
2500	90.68	80.14	1.6914	0.5452
3000	93.30	89.24	2.2316	0.5523

TABLE 10. Properties of ethylene as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
250 K	− 201.59	8.60	0.0895	0.0002
300	− 138.03	10.37	0.1281	0.0966
0 °C	− 167.98	9.43	0.1067	0.0483
20	− 144.94	10.13	0.1225	0.0849
40	− 125.94	10.82	0.1392	0.1178
60	− 110.02	11.49	0.1568	0.1475
80	− 96.47	12.15	0.1751	0.1745
100	− 84.81	12.79	0.1943	0.1990
150	− 61.70	14.34	0.2455	0.2516
200	− 44.56	15.81	0.3013	0.2945
250	− 31.36	17.22	0.3614	0.3299
300	− 20.90	18.58	0.4256	0.3596
350	− 12.43	19.88	0.4937	0.3847
400	− 5.45	21.14	0.5656	0.4061
450	0.37	22.35	0.6411	0.4245
500	5.29	23.53	0.7202	0.4404
600	13.06	25.78	0.8888	0.4662
700	18.84	27.92	1.0705	0.4859
800	23.22	29.96	1.2649	0.5011
900	26.59	31.92	1.4716	0.5130
1000	29.20	33.80	1.6901	0.5222
1500	35.98	42.39	2.9512	0.5447
2000	38.59	50.02	4.4747	0.5482

TABLE 11. Properties of ethane as a function of temperature

T K or °C	B 10^{-3} m^3/kmol	η μPa s	D(1.013 bar) 10^{-4} m^2/s	α_0
250 K	− 264.91	7.77	0.0753	0.0057
300	− 183.36	9.36	0.1078	0.1015
0 °C	− 221.86	8.52	0.0898	0.0535
20	− 192.25	9.15	0.1031	0.0899
40	− 167.77	9.76	0.1171	0.1227
60	− 147.18	10.37	0.1319	0.1522
80	− 129.63	10.96	0.1473	0.1789
100	− 114.48	11.53	0.1634	0.2033
150	− 84.36	12.93	0.2064	0.2555
200	− 61.92	14.25	0.2532	0.2981
250	− 44.57	15.52	0.3037	0.3332
300	− 30.78	16.74	0.3575	0.3627
350	− 19.59	17.91	0.4147	0.3875
400	− 10.34	19.04	0.4750	0.4087
450	− 2.61	20.13	0.5384	0.4269
500	3.92	21.19	0.6048	0.4426
600	14.27	23.21	0.7462	0.4681
700	21.97	25.13	0.8987	0.4876
800	27.80	26.97	1.0618	0.5025
900	32.28	28.73	1.2353	0.5142
1000	35.75	30.42	1.4186	0.5232
1500	44.64	38.14	2.4769	0.5450
2000	47.93	45.00	3.7554	0.5481

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Appendix A: Material and Physical Constants Including Scaling Factors

TABLE A1. Universal constants[a]

Boltzmann constant	$k = 1.380\,662\times10^{-23} J\,K^{-1}$
Avogadro constant	$N_A = 6.022\,045\times10^{23}$ mol^{-1}
Universal gas constant	$R = 8.314\,41$ J mol^{-1} K^{-1}

[a] Reference 15.

TABLE A2. Molecular weights[a] (average isotopic composition, kg/kmol)

N_2	28.013 4
O_2	31.998 8
NO	30.006 1
CO	28.010 6
CO_2	44.010 0
N_2O	44.012 8
CH_4	16.043 03
CF_4	88.004 8
SF_6	146.054
C_2H_4	28.054 18
C_2H_6	30.070 12

[a] Reference 16.

TABLE A3. Effective spherical scaling parameters σ and ϵ, and high-temperature dimensionless scaling parameters $\rho^* = \rho/\sigma$ and $V_0^* = V_0/\epsilon$

	σ(nm)	ϵ/k(K)	ρ^*	V_0^{*a}
N_2	0.3652	98.4	0.1080	5.308(+ 4)
O_2	0.3407	121.1	0.0745	1.322(+ 6)
NO	0.3474	125.0	0.0883	2.145(+ 5)
CO	0.3652	98.4	0.1080	5.308(+ 4)
CO_2	0.3769	245.3	0.0720	2.800(+ 6)
N_2O	0.3703	266.8	0.0730	2.600(+ 6)
CH_4	0.3721	161.4	0.0698	3.066(+ 6)
CF_4	0.4579	156.5	0.0200	1.460(+ 19)
SF_6	0.5252	207.7	0.0500	4.067(+ 8)
C_2H_4	0.4071	244.3	···	···
C_2H_6	0.4371	241.9	···	···

[a] Values in parentheses are the powers of 10 by which the entries are to be multiplied.

TABLE A4. Dimensionless material parameters for the calculation of the nonspherical contributions to second virial coefficients

	$\mu^{*\,a}$	$\Theta^{*\,b}$	$\alpha^{*\,d}$	κ^f	$C_6^{*\,g}$
N_2	0	0.47[c]	0.0357	0.131	2.18
O_2	0	0.141	0.0397	0.229	2.27
NO	0.180	0.61	0.0408	0.162	2.20
CO	0.138	0.84	0.0404	0.090	2.63[h]
CO_2	0	0.85	0.0547	0.268	1.89[i]
N_2O	0.122	0.59	0.0607	0.329	1.86
CH_4	0	0	0.0503	0	2.10[j]
CF_4	0	0	0.0402[e]	0	1.35[k]
SF_6	0	0	0.0452[e]	0	1.51[l]
C_2H_4	0	0.33[c]	0.0631	0.143	2.13[m]
C_2H_6	0	0.11[c]	0.0529	0.058	1.57[n]

Dipole moment $\mu^* = \mu_0/(\epsilon\sigma^3)^{1/2}$
Quadrupole moment $\Theta^* = \Theta/(\epsilon\sigma^5)^{1/2}$
Dipole polarizability $\alpha^* = \bar{\alpha}_d/\sigma^3$
$\bar{\alpha}_d = \frac{1}{3}(\alpha_d^{\parallel} + 2\alpha_d^{\perp})$
Polarizability anisotropy $\kappa = (\alpha_d^{\parallel} - \alpha_d^{\perp})/3\bar{\alpha}_d$
Dispersion coefficient $C_6^* = \bar{C}_6/\epsilon\sigma^6$

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[k] Estimated from the Slater–Kirkwood formula with an effective number of oscillators, $N = 8$ (2 electrons in each of 4 single C–F bonds).

[l] Calculated from the C_6 values for SF_6–Ne by R. T. Pack, E. Piper, G. A. Pfeffer, and J. P. Toennies, J. Chem. Phys. **80**, 4940 (1984) and for SF_6–Ar by R. T. Pack, J. J. Valentine, and J. B. Cross, J. Chem. Phys. **77**, 5486 (1982), using the combination rule discussed by H. L. Kramer and D. R. Herschbach, J. Chem. Phys. **53**, 2792 (1970).

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Appendix B: Correlation Equations for Functionals

Collision Integrals

$\Omega^{(2,2)*}$,

$1 \leqslant T^* \leqslant 10$,

$$\Omega^{(2,2)*} = \exp[0.466\,41 - 0.569\,91 \ln T^* + 0.195\,91(\ln T^*)^2 - 0.038\,79(\ln T^*)^3 + 0.002\,59(\ln T^*)^4]. \qquad \text{(B1a)}$$

$T^* \geqslant 10$,

$$\Omega^{(2,2)*} = (\rho^*)^2\alpha^2[1.04 + a_1(\ln T^*)^{-1} + a_2(\ln T^*)^{-2} + a_3(\ln T^*)^{-3} + a_4(\ln T^*)^{-4}], \qquad \text{(B1b)}$$

where

$$a_1 = 0,$$

$$a_2 = -33.0838 + (\alpha_{10}\rho^*)^{-2}[20.0862 + (72.1059/\alpha_{10}) + (8.276\,48/\alpha_{10})^2],$$

$$a_3 = 101.571 - (\alpha_{10}\rho^*)^{-2}[56.4472 + (286.393/\alpha_{10}) + (17.7610/\alpha_{10})^2],$$

$$a_4 = -87.7036 + (\alpha_{10}\rho^*)^{-2}[46.3130 + (277.146/\alpha_{10}) + (19.0573/\alpha_{10})^2],$$

in which $\alpha_{10} = \ln(V_0^*/10)$ is the value of $\alpha = \ln V_0^* - \ln T^*$ at the matching point of $T^* = 10$. These expressions are identical to those of Ref. 2.

$\Omega^{(1,1)*}$,

$1 \leqslant T^* \leqslant 10$,

$$\Omega^{(1,1)*} = \exp[0.295\,402 - 0.510\,069 \ln T^* + 0.189\,395\,(\ln T^*)^2 - 0.045\,427(\ln T^*)^3 + 0.003\,7928(\ln T^*)^4]. \qquad \text{(B2a)}$$

$T^* \geqslant 10$,

$$\Omega^{(1,1)*} = (\rho^*)^2\alpha^2[0.89 + b_2(T^*)^{-2} + b_4(T^*)^{-4} + b_6(T^*)^{-6}], \qquad \text{(B2b)}$$

where

$$b_2 = -267.00 + (\alpha_{10}\rho^*)^{-2}[201.570 + (174.672/\alpha_{10}) + (7.369\,16/\alpha_{10})^2],$$

$$b_4 = 26\,700 - (\alpha_{10}\rho^*)^{-2}[19.2265 + (27.6938/\alpha_{10}) + (3.295\,59/\alpha_{10})^2] \times 10^3,$$

$$b_6 = -8.90 \times 10^5 + (\alpha_{10}\rho^*)^{-2}[6.310\,13 + (10.2266/\alpha_{10}) + (2.330\,33/\alpha_{10})^2] \times 10^5,$$

in which $\alpha_{10} = \ln(V_0^*/10)$ is the value of $\alpha = \ln V_0 - \ln T^*$ at the matching point of $T^* = 10$. Equation (B2b) is identical to the corresponding expression of Ref. 2, but Eq. (B2a) has been adjusted slightly to be a better fit of the data near 300 K; it gives $\Omega^{(1,1)*}$ about 3% smaller at $T^* = 3$.

Second Virial Coefficients

$$B^* = B_0^* + B_{ns}^*, \qquad \text{(B3)}$$

B_0^*,

$1 \leqslant T^* \leqslant 10$,

$$B_0^* = -(T^*)^{1/2} \exp(1/T^*)[c_0 + c_1 \ln T^* + c_2(\ln T^*)^2 + c_3(\ln T^*)^3 + c_4(\ln T^*)^4], \qquad \text{(B4a)}$$

where the coefficients c_i are given in Table B1.

$T^* \geqslant 10$,

$$B_0^* = \beta\,[1 + d_2(\ln T^*)^{-2} + d_4(\ln T^*)^{-4} + d_6(\ln T^*)^{-6}], \qquad \text{(B4b)}$$

where

$$\beta = (\rho^*)^3[(\alpha + \gamma)^3 + (\pi^2/2)(\alpha + \gamma) + 2.404\,11],$$

$$\alpha = \ln V_0^* - \ln T^*$$

$\gamma = 0.577\,215...$ is Euler's constant,

and

$$d_2 = -15.9057 + (9.859\,58/\beta_{10}) + [(\rho^*)^3/\beta_{10}^2][25.6607(\alpha_{10} + \gamma)^2 - 9.737\,66(\alpha_{10} + \gamma) + 42.2102] + 3.245\,89[(\rho^*)^2/\beta_{10}]^3[3(\alpha_{10} + \gamma)^2 + \pi^2/2]^2,$$

$$d_4 = 84.3304 - (61.9124/\beta_{10}) + [(\rho^*)^3/\beta_{10}^2][-227.258(\alpha_{10} + \gamma)^2 + 103.256(\alpha_{10} + \gamma) - 373.824] - 34.4187[(\rho^*)^2/\beta_{10}]^3[3(\alpha_{10} + \gamma)^2 + \pi^2/2]^2,$$

$$d_6 = -149.037 + (119.937/\beta_{10}) + [(\rho^*)^3/\beta_{10}^2][483.571(\alpha_{10} + \gamma)^2 - 273.727(\alpha_{10} + \gamma) + 795.442] + 91.2423[(\rho^*)^2/\beta_{10}]^3[3(\alpha_{10} + \gamma)^2 + \pi^2/2]^2,$$

in which β_{10} is the value of β and α_{10} is the value of α at the matching point of $T^* = 10$.

B_{ns}^*,

$T^* \geqslant 1$,

$$B_{ns}^* = B_{ns}^*(\mu\mu) + B_{ns}^*(\mu\Theta) + B_{ns}^*(\Theta\Theta) + \cdots + B_{ns}^*(\mu,\text{ind}\,\mu) + B_{ns}^*(\mu\Theta,\text{ind}\,\mu) + B_{ns}^*(\Theta,\text{ind}\,\mu) + \cdots + B_{ns}^*(C_6\text{anis}) + \cdots + \text{cross terms}. \qquad \text{(B5)}$$

TABLE B1. Coefficients of Eq. (B4a) for the computation of the functional B_0^*

	c_0	c_1	c_2	c_3	c_4
Noble gases	0.746 85	− 1.038 40	0.316 34	0.020 96	− 0.014 98
N_2, CO, O_2, NO	0.968 43	− 1.344 24	0.464 05	− 0.006 89	− 0.013 58
CO_2	0.826 01	− 1.390 73	0.685 81	− 0.126 53	0.005 43
N_2O	0.868 75	− 1.286 42	0.501 53	− 0.039 49	− 0.007 67
CH_4	0.899 21	− 1.250 84	0.420 71	0.000 59	− 0.013 84
CF_4	1.062 88	− 1.494 08	0.552 40	− 0.029 79	− 0.011 38
SF_6	1.218 52	− 1.917 94	0.928 50	− 0.167 63	0.006 73
C_2H_4	0.904 34	− 1.397 38	0.605 82	− 0.078 96	− 0.002 38
C_2H_6	0.987 55	− 1.475 80	0.613 82	− 0.068 80	− 0.004 84

Explicit formulas for the various contributions to B_{ns}^* are given in Ref. 14 as power series in $(T^*)^{-1}$, together with numerical tables of auxiliary functions used in their computation.

Appendix C: General Formulas

Viscosity η

$$\eta = \frac{5}{16}\left(\frac{mkT}{\pi}\right)^{1/2} \frac{f_\eta}{\sigma^2\Omega^{(2,2)*}}, \tag{C1}$$

$$f_\eta = 1 + (3/196)\,(8E^* - 7)^2. \tag{C2}$$

Self-diffusion Coefficient D

$$D = \frac{3}{8P}\left(\frac{k^3T^3}{\pi m}\right)^{1/2} \frac{f_D}{\sigma^2\Omega^{(1,1)*}}, \tag{C3}$$

where P is the pressure, and

$$f_D = 1 + \frac{1}{8}\frac{(6C^* - 5)^2}{2A^* + 5}. \tag{C4}$$

Isotopic Thermal Diffusion Factor α_0

$$\alpha_0 = \frac{15}{2}\frac{(6C^* - 5)(2A^* + 5)}{A^*(16A^* - 12B^* + 55)}(1 + \kappa_0), \tag{C5}$$

$$\kappa_0 = \frac{1}{9}(7 - 8\text{E}^*)\left[\frac{2A^*}{(35/4) + 7A^* + 4F^*}\left(H^* + \frac{[A^*(7 - 8E^*) - 7(6C^* - 5)][(35/8) + 28A^* - 6F^*]}{42A^*(2A^* + 5)}\right)\right.$$
$$\left. - \frac{5}{7}\left(H^* + \frac{7}{5}\frac{(6C^* - 5)}{(2A^* + 5)} - \frac{3}{10}(7 - 8E^*)\right)\right\}. \tag{C5a}$$

Reference 1 (Table VII) lists values of κ_0, which are very close to those implied in the above equation.

Auxiliary Functions

$$A^* = \Omega^{(2,2)*}/\Omega^{(1,1)*}, \tag{C6}$$

$$B^* = [5\Omega^{(1,2)*} - 4\Omega^{(1,3)*}]/\Omega^{(1,1)*}$$
$$= 1 + 3C^* - 3(C^*)^2 - \frac{(T^*)^2}{3}\frac{d^2\ln\Omega^{(1,1)*}}{dT^{*2}}$$
$$= 4C^* - 3(C^*)^2 - \frac{1}{3}\frac{d^2\ln\Omega^{(1,1)*}}{d(\ln T^*)^2}, \tag{C7}$$

$$C^* = \frac{\Omega^{(1,2)*}}{\Omega^{(1,1)*}} = 1 + \frac{T^*}{3}\frac{d\ln\Omega^{(1,1)*}}{dT^*}, \tag{C8}$$

$$E^* = \frac{\Omega^{(2,3)*}}{\Omega^{(2,2)*}} = 1 + \frac{T^*}{4}\frac{d\ln\Omega^{(2,2)*}}{dT^*}, \tag{C9}$$

$$F^* = \frac{\Omega^{(3,3)*}}{\Omega^{(1,1)*}} = 0.9543 + 0.001\,24\,T^*, \tag{C10}$$

$$H^* = (3B^* + 6C^* - 35/4)(6C^* - 5)^{-1}. \tag{C11}$$

The numerical expression for F* is a correlation from Ref. 1; the other expressions are definitions and recursion relations.

Second Virial Coefficient B

$$B = \tfrac{2}{3}N_A\pi\sigma^3B^*. \tag{C12}$$

Appendix D: Deviation Plots (Figs. 4–43)

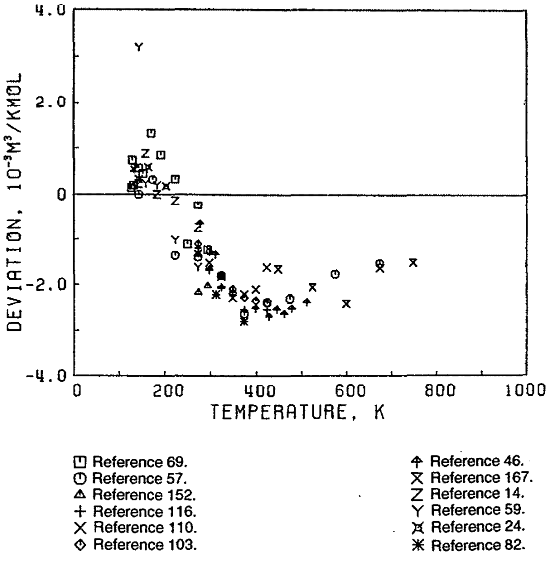

FIG. 4. Deviation plot for the second virial coefficient of nitrogen, primary data.

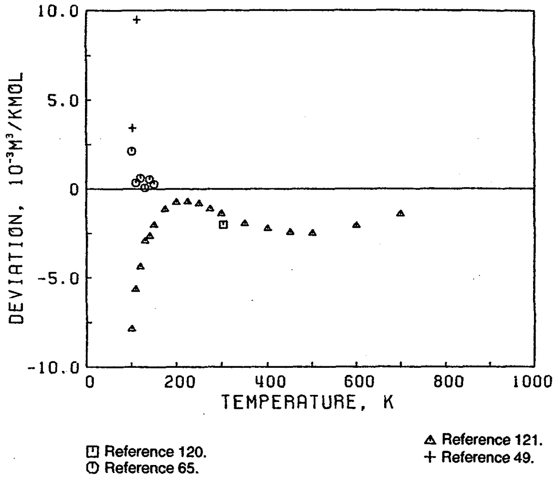

FIG. 5. Deviation plot for the second virial coefficient of nitrogen, secondary data.

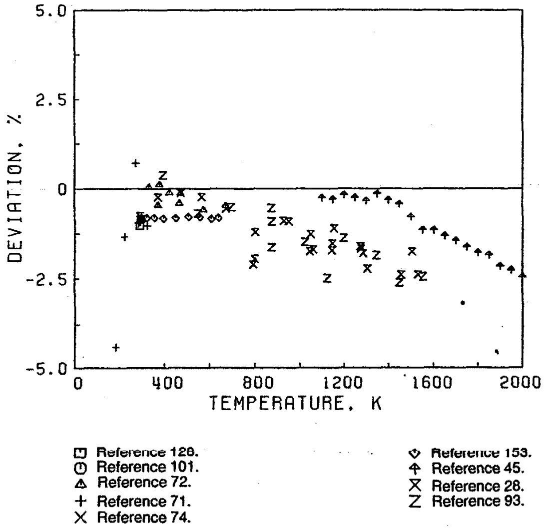

FIG. 6. Deviation plot for the viscosity of nitrogen, primary data.

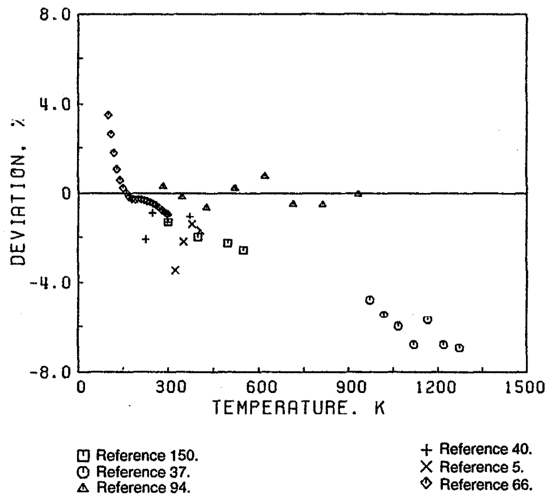

FIG. 7. Deviation plot for the viscosity of nitrogen, secondary data.

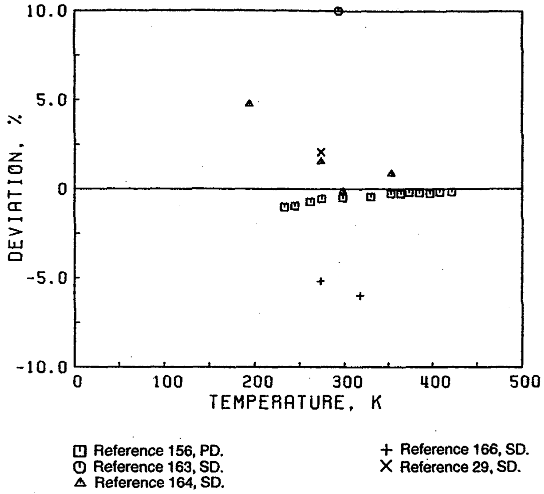

FIG. 8. Deviation plot for the self-diffusion coefficient of nitrogen, primary and secondary data.

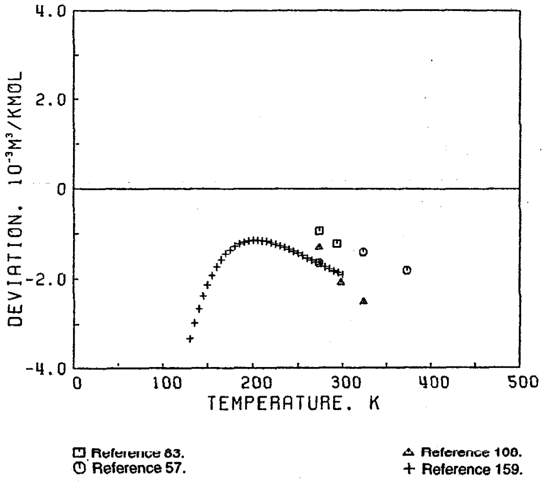

FIG. 9. Deviation plot for the second virial coefficient of oxygen, primary data.

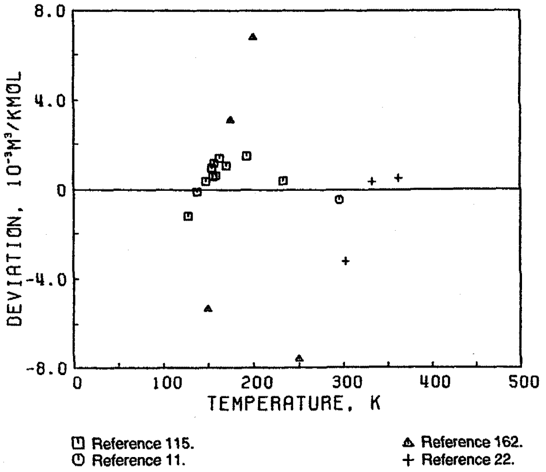

FIG. 10. Deviation plot for the second virial coefficient of oxygen, secondary data.

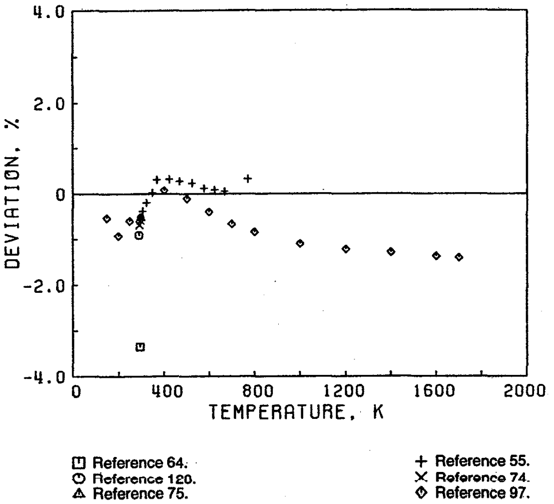

FIG. 11. Deviation plot for the viscosity of oxygen, primary data.

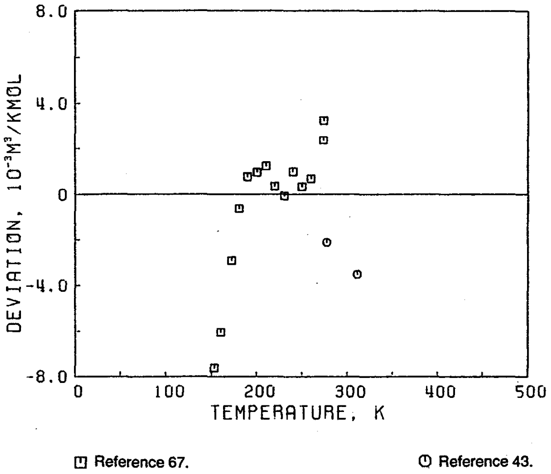

FIG. 14. Deviation plot for the second virial coefficient of nitric oxide, secondary data.

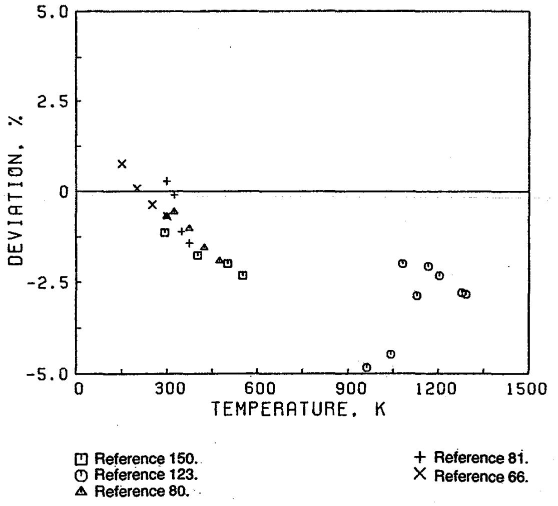

FIG. 12. Deviation plot for the viscosity of oxygen, secondary data.

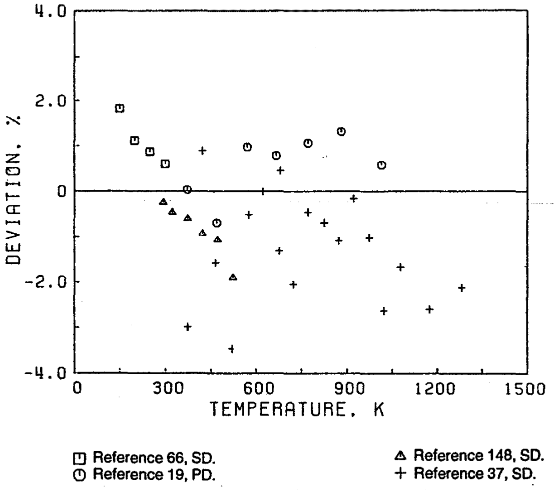

FIG. 15. Deviation plot for the viscosity of nitric oxide, primary and secondary data.

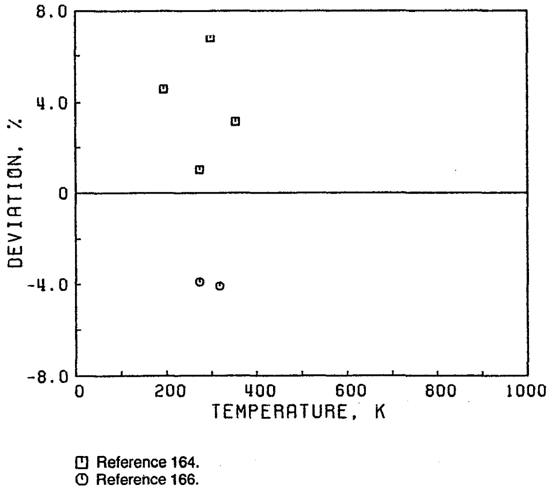

FIG. 13. Deviation plot for the self-diffusion coefficient of oxygen, secondary data.

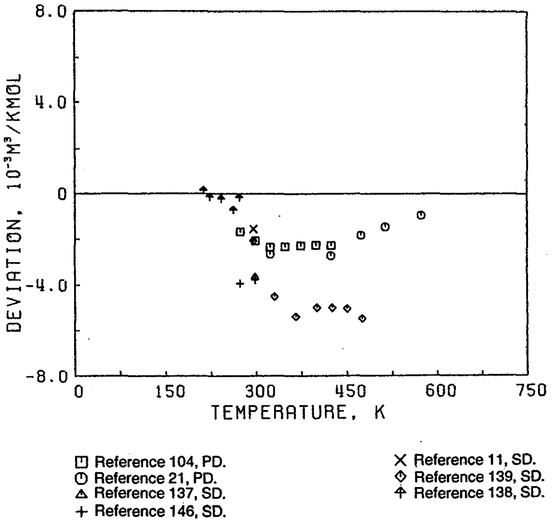

FIG. 16. Deviation plot for the second virial coefficient of carbon monoxide, primary and secondary data.

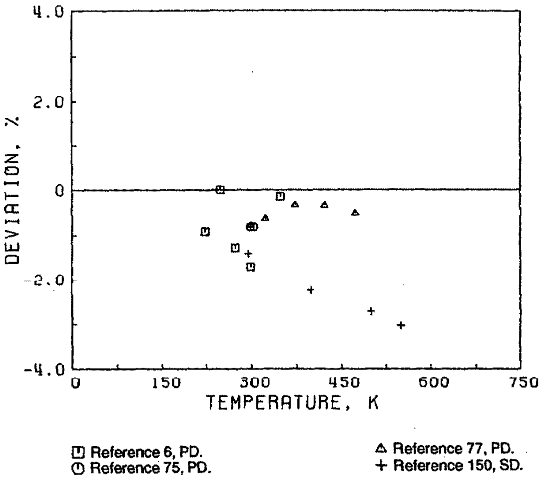

FIG. 17. Deviation plot for the viscosity of carbon monoxide, primary and secondary data.

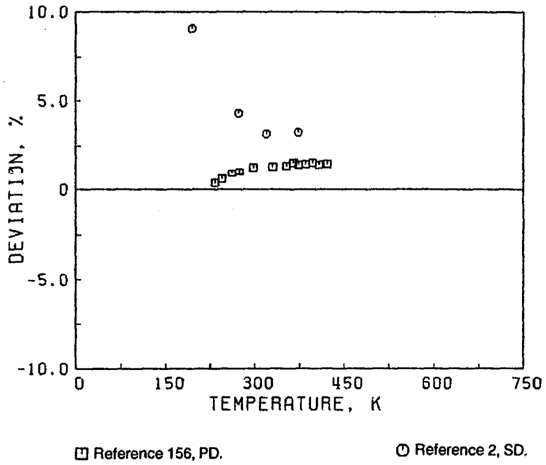

FIG. 18. Deviation plot for the self-diffusion coefficient of carbon monoxide, primary and secondary data.

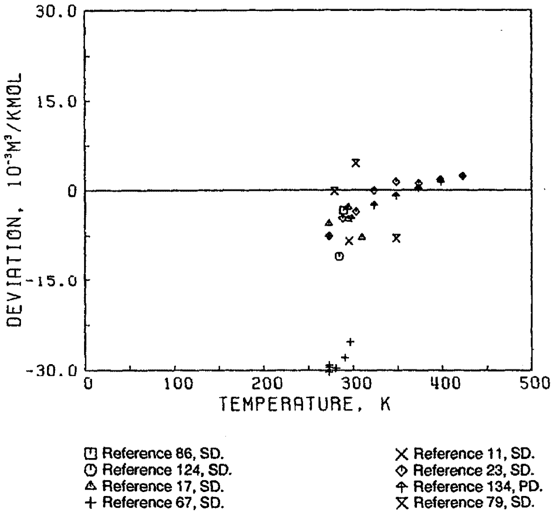

FIG. 19. Deviation plot for the second virial coefficient of nitrous oxide, primary and secondary data.

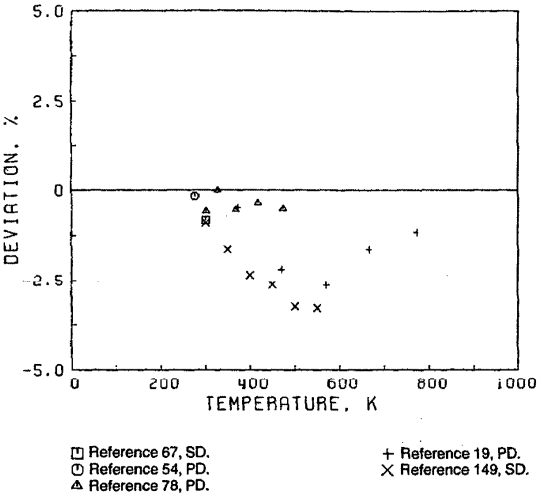

FIG. 20. Deviation plot of the viscosity of nitrous oxide, primary and secondary data.

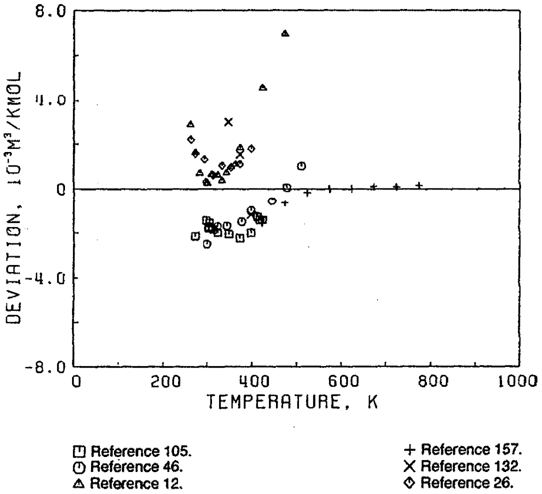

FIG. 21. Deviation plot for the second virial coefficient of carbon dioxide, primary data.

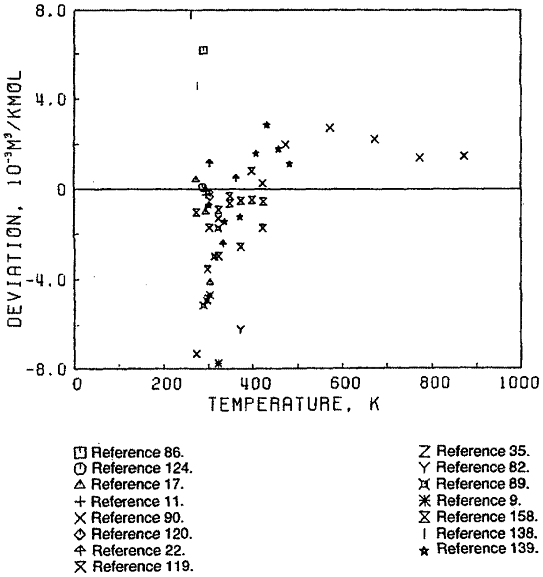

FIG. 22. Deviation plot for the second virial coefficient of carbon dioxide, secondary data.

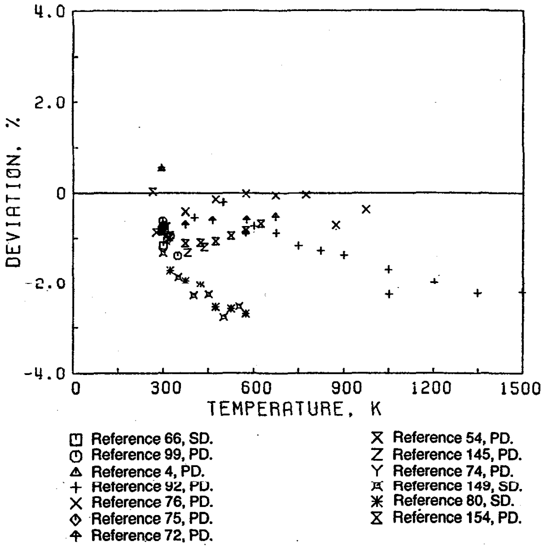

FIG. 23. Deviation plot for the viscosity of carbon dioxide, primary and secondary data.

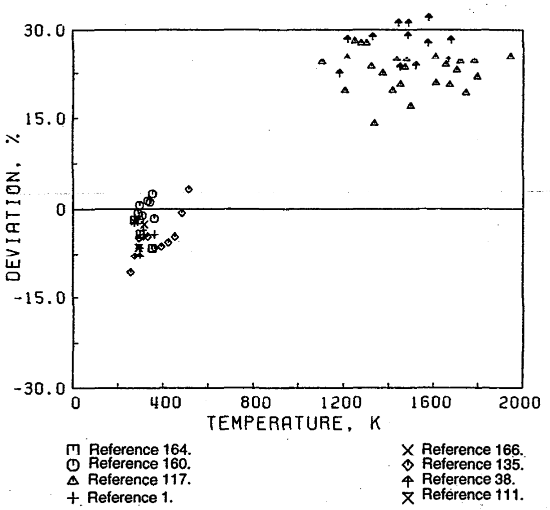

FIG. 24. Deviation plot for the self-diffusion coefficient of carbon dioxide, secondary data.

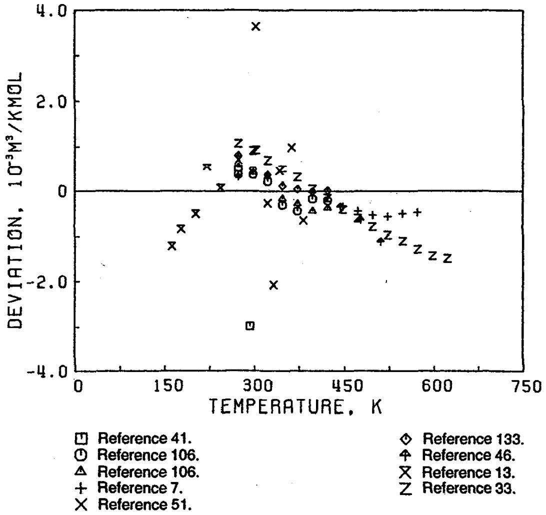

FIG. 25. Deviation plot for the second virial coefficient of methane, primary data.

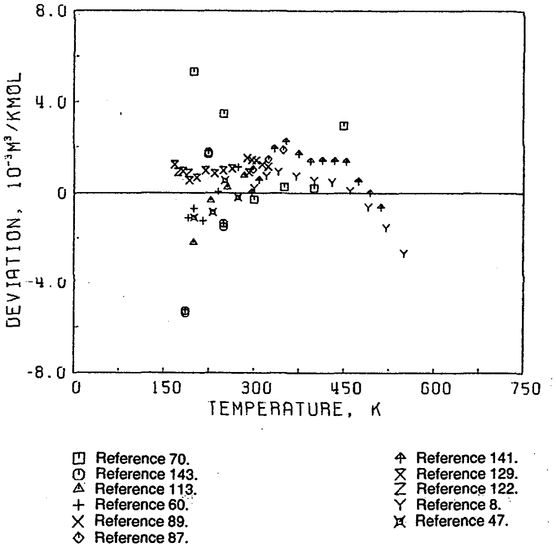

FIG. 26. Deviation plot for the second virial coefficient of methane, secondary data.

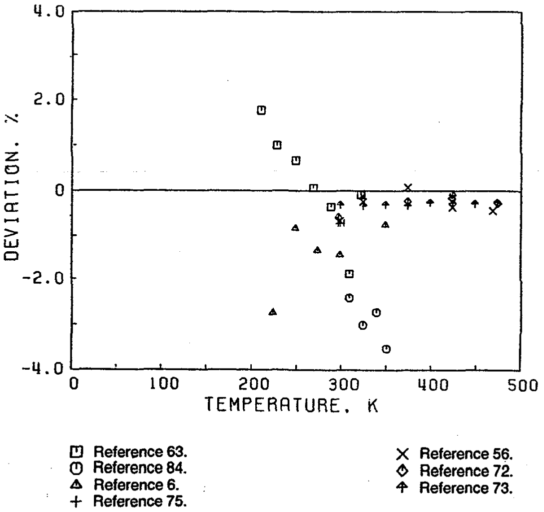

FIG. 27. Deviation plot for the viscosity of methane, primary data.

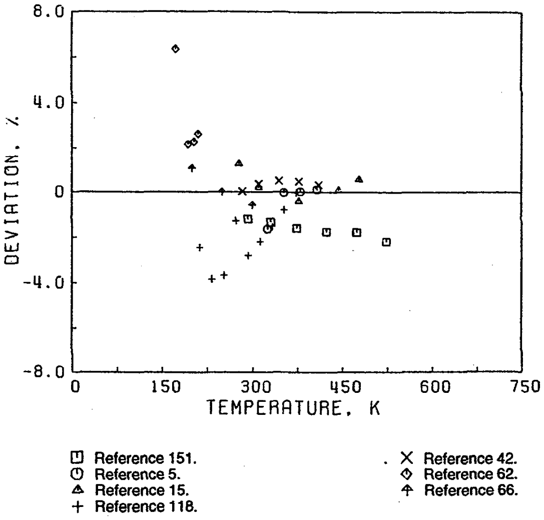

FIG. 28. Deviation plot for the viscosity of methane, secondary data.

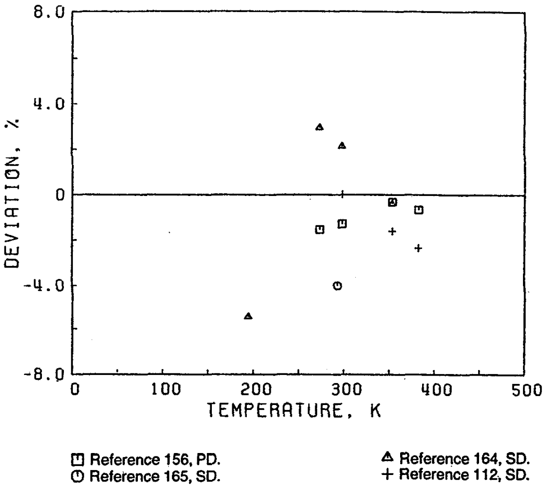

FIG. 29. Deviation plot for the self-diffusion coefficient of methane, primary and secondary data.

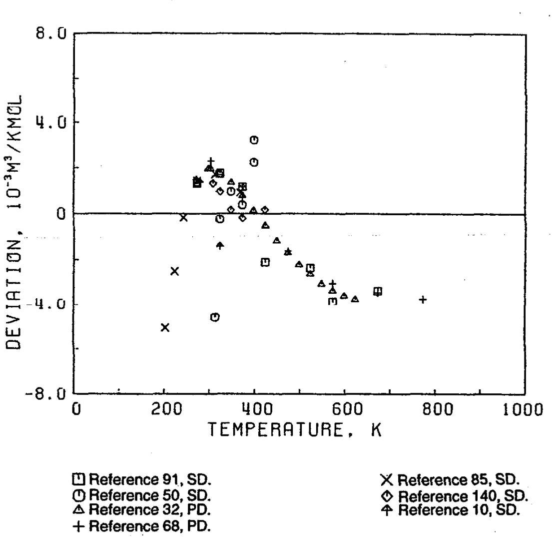

FIG. 30. Deviation plot for the second virial coefficient of carbon tetrafluoride, primary and secondary data.

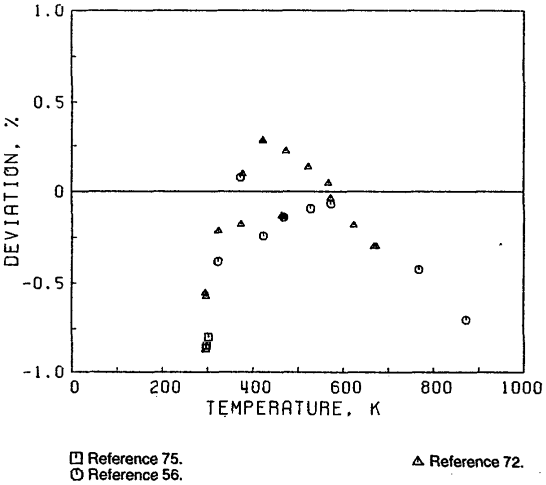

FIG. 31. Deviation plot for the viscosity of carbon tetrafluoride, primary data.

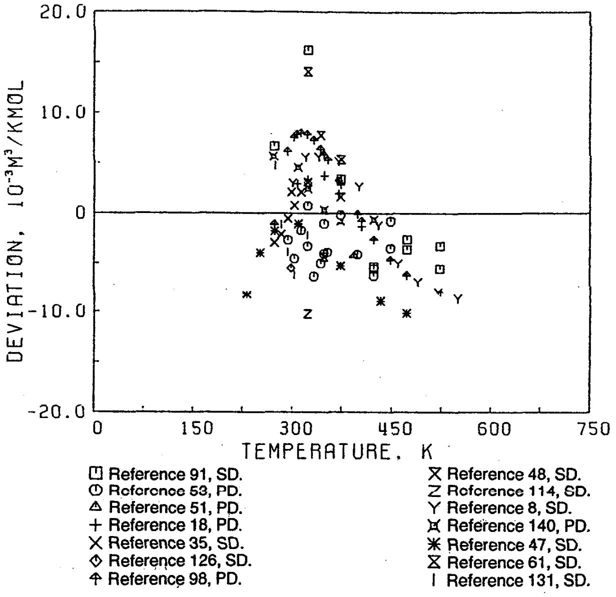

FIG. 32. Deviation plot for the second virial coefficient of sulfur hexafluoride, primary and secondary data.

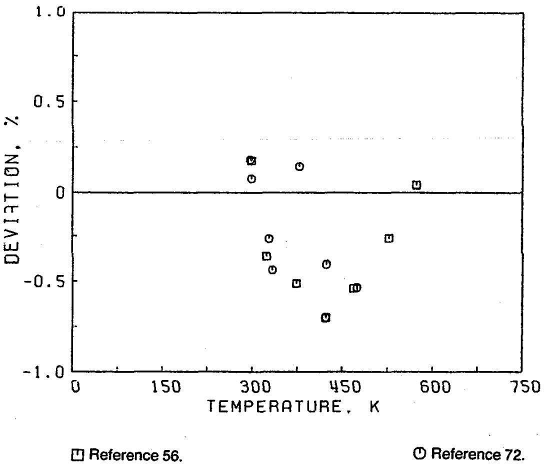

FIG. 33. Deviation plot for the viscosity of sulfur hexafluoride, primary data.

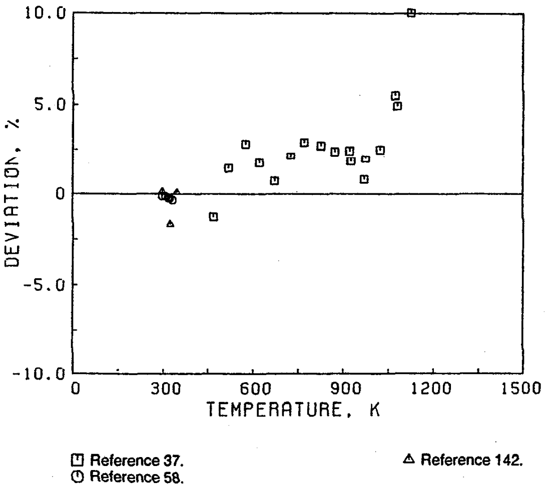

FIG. 34. Deviation plot for the viscosity of sulfur hexafluoride, secondary data.

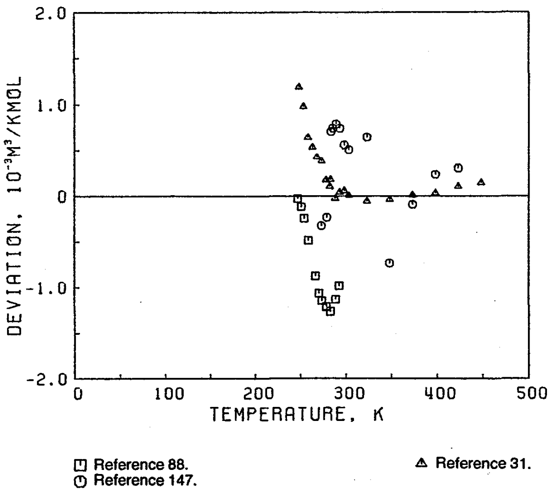

FIG. 35. Deviation plot for the second virial coefficient of ethylene, primary data.

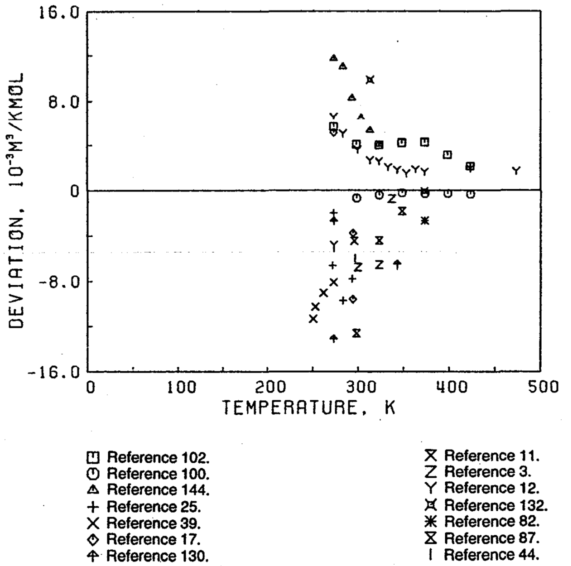

FIG. 36. Deviation plot for the second virial coefficient of ethylene, secondary data.

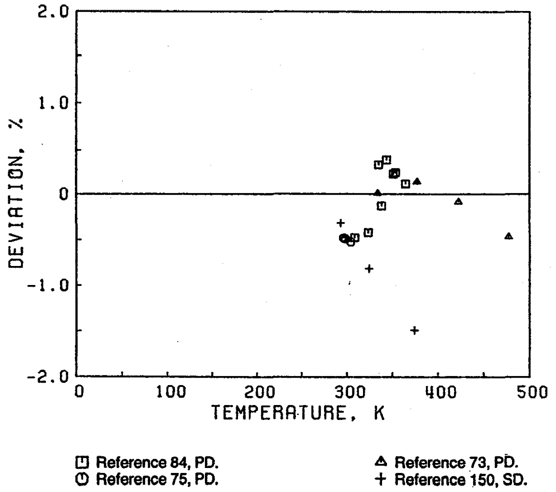

FIG. 37. Deviation plot for the viscosity of ethylene, primary and secondary data.

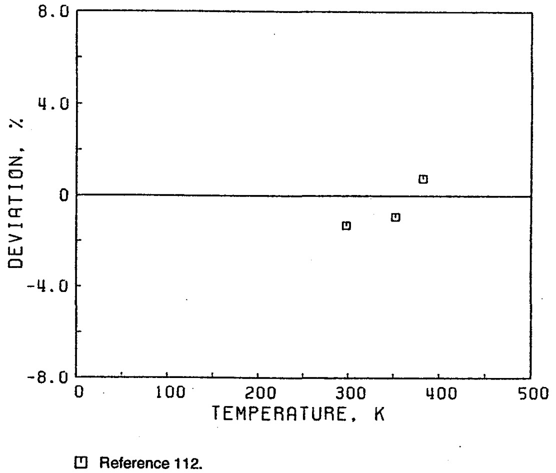

FIG. 38. Deviation plot for the self-diffusion coefficient of ethylene, secondary data.

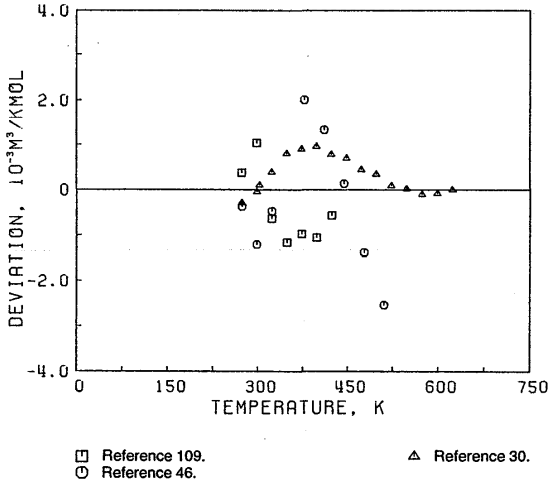

FIG. 39. Deviation plot for the second virial coefficient of ethane, primary data.

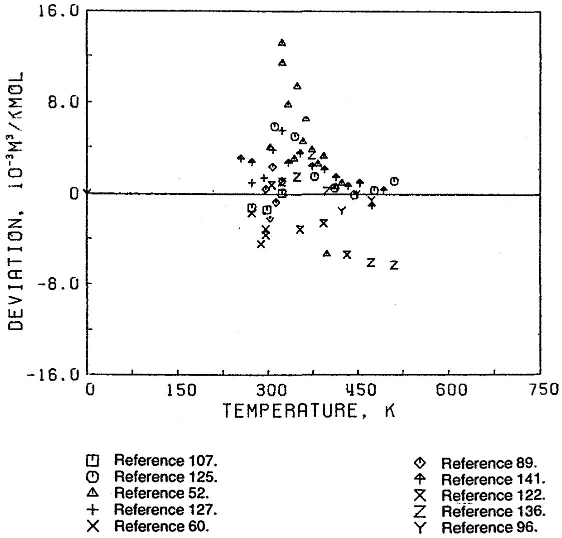

FIG. 40. Deviation plot for the second virial coefficient of ethane, secondary data.

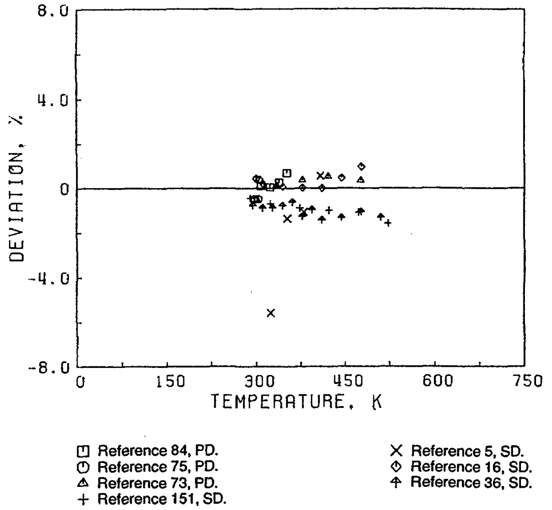

FIG. 41. Deviation plot for the viscosity of ethane, primary and secondary data.

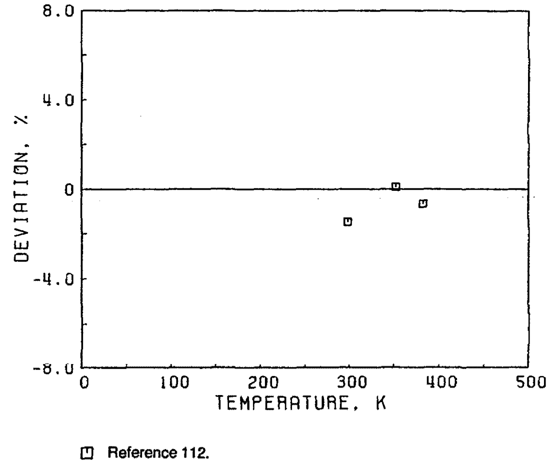

FIG. 42. Deviation plot for the self-diffusion coefficient of ethane, secondary data.

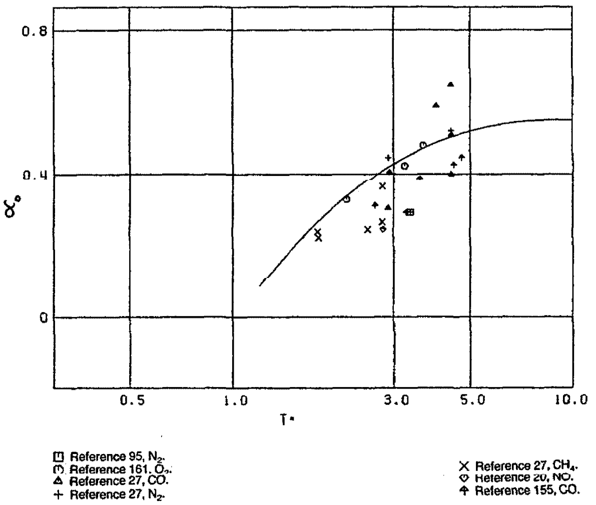

FIG. 43. Isotopic thermal diffusion factor of nitrogen, oxygen, nitric oxide, carbon monoxide, and methane.

Appendix E: References for Deviation Plots (Figs. 4–43)

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