

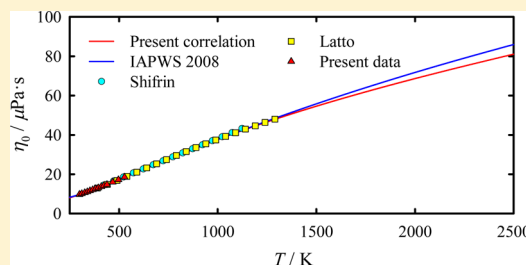
The Viscosity of Dilute Water Vapor Revisited: New Reference Values from Experiment and Theory for Temperatures between (250 and 2500) K

Robert Hellmann* and Eckhard Vogel

Institut für Chemie, Universität Rostock, 18059 Rostock, Germany

S Supporting Information

ABSTRACT: Previously reported as well as unpublished experimental data for the viscosity of dilute water vapor in the temperature range from (297 to 528) K, which were obtained using an oscillating-disk viscometer, have been re-evaluated and extrapolated to the limit of zero density. The relative combined expanded ($k = 2$) uncertainty of the re-evaluated data is 0.2 % at room temperature (297 K to 302 K), 0.4 % at higher temperatures up to 450 K, and 1.0 % at temperatures above 450 K. The classical kinetic theory of molecular gases has been applied to compute the viscosity in the limit of zero density for temperatures between (250 and 2500) K using a highly accurate ab initio potential for the H_2O molecule pair. In the temperature range from (311 to 438) K, the experimental zero-density data differ by only about +0.1 % from the calculated values. A new correlation for the zero-density limit, based on both the experimental data and the theoretically calculated values, is proposed. The relative combined expanded ($k = 2$) uncertainty of the correlation is estimated to be 0.4 % between (300 and 500) K, increasing to 0.8 % at 250 K and 2.0 % at 2500 K. The new correlation represents a significant improvement over the current IAPWS zero-density correlation.



1. INTRODUCTION

A study of the viscosity of water vapor resulting from ten series of measurements by means of an all-quartz oscillating-disk viscometer at temperatures between (298 and 438) K was reported by Teske et al. in 2005.¹ Because it was difficult to find out whether some further experimental points measured at still higher temperatures were influenced by potential reactions between water vapor and quartz glass, these and further data, taken after the highest temperature had been attained, were left out in that report. Moreover, the data of four additional series of measurements carried out by Teske et al. were not published in 2005 because they did not offer substantially different results.

In a subsequent paper,² we calculated transport and relaxation properties of dilute water vapor using the kinetic theory of polyatomic gases³ and four different intermolecular potential energy surfaces. The temperature dependence of the computed values for the shear viscosity in the zero-density limit, η_0 , was consistent with that of the published data of Teske et al.¹

Therefore, improved theoretically calculated viscosity values should enable to assess the reliability of the unpublished data of Teske et al. Furthermore, all measured data of Teske et al. should be re-evaluated because the viscometer was calibrated originally with an experimentally based reference value for the zero-density viscosity of argon at room temperature, which was recommended by Kestin et al. in 1972⁴ and is nowadays out of date.

2. EXPERIMENTAL AND COMPUTATIONAL METHODS

2.1. Measurements with the Oscillating-Disk Viscometer. In the present paper, the measurements of Teske et al.¹ were re-evaluated with regard to the calibration of the viscometer. For that purpose, the Newell constant C_N of the respective evaluation procedure⁵ was redetermined on the basis of a new viscosity value at room temperature theoretically calculated by Vogel et al.⁶ using an ab initio potential energy curve for the argon atom pair⁷ and the kinetic theory of dilute monatomic gases. The relative uncertainty of this value was assumed to be 0.1 %. A comparison between another computed viscosity value for argon obtained by Mehl, though unpublished, and that by Vogel et al., shown in Figure 7.2b of ref 8, makes it obvious that the relative uncertainty of the theoretically calculated values could reasonably be lowered to 0.07 %. The old experimentally based reference value of Kestin et al.⁴ and the new theoretical value of Vogel et al. used for the recalibration disagree at 298.15 K by 0.217 %, $\eta_{0,\text{Ar,Kestin}} = 22.601 \mu\text{Pa}\cdot\text{s}$ and $\eta_{0,\text{Ar,Vogel}} = 22.552 \mu\text{Pa}\cdot\text{s}$. Since the measurements were not performed exactly at 298.15 K and of course not at zero density, coefficients of the temperature and density dependencies of the viscosity of argon are required

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Table 1. Coefficients for the Limit of Zero Density, η_0 , and for the Initial Density Dependence, η_1 , of the Viscosity Resulting from the Re-Evaluated Quasiexperimental Isotherms of the Measurements of Teske et al.¹ on Water Vapor

T K	n^a	$\eta_0 \pm \sigma_{\eta_0}$ $\mu\text{Pa}\cdot\text{s}$	$\eta_{0,\text{RF}}$ $\mu\text{Pa}\cdot\text{s}$	$\eta_1 \pm \sigma_{\eta_1}$ $\mu\text{Pa}\cdot\text{s}\cdot\text{m}^3\cdot\text{kg}^{-1}$	$10^3\cdot\sigma_{\eta}$ $\mu\text{Pa}\cdot\text{s}$
298.49	3	9.718 ± 0.015	9.687^b	-1.871 ± 0.604	2.72
311.38	6	10.126 ± 0.007		-0.148 ± 0.192	5.23
326.23	9	10.644 ± 0.003		-0.196 ± 0.034	4.81
339.09	12	11.088 ± 0.004		-0.117 ± 0.008	7.59
352.64	14	11.576 ± 0.002		-0.228 ± 0.011	4.90
366.83	14	12.088 ± 0.003		-0.213 ± 0.016	6.92
381.30	14	12.618 ± 0.003		-0.200 ± 0.016	6.87
394.89	14	13.122 ± 0.004		-0.134 ± 0.023	9.70
409.16	14	13.661 ± 0.005		-0.036 ± 0.026	11.32
423.18	14	14.204 ± 0.005		0.006 ± 0.026	11.01
438.36	14	14.796 ± 0.006		0.158 ± 0.030	12.68
467.47	14	15.959 ± 0.009		0.393 ± 0.049	21.13
496.79	14	17.175 ± 0.017		0.726 ± 0.091	38.92
527.46 ^c	3	18.484 ± 0.100		2.099 ± 1.076	84.38
299.51 ^d	3	9.747 ± 0.004	9.731^b	-1.121 ± 0.148	0.66
381.55 ^d	14	12.626 ± 0.003		-0.046 ± 0.019	7.97

^aNumber of quasiexperimental points included in the fit of eq 2. ^bValue resulting by means of the Rainwater–Friend theory to correct for the initial density dependence of the viscosity. ^cOnly three data points at the highest temperature. ^dRemeasurements at lower temperatures after the highest temperature had been attained.

for the calibration. They were taken from refs 6 and 4, $(\partial\eta/\partial T)_\rho = 0.0635 \mu\text{Pa}\cdot\text{s}\cdot\text{K}^{-1}$ and $(\partial\eta/\partial\rho)_T = 11.099 \text{ nPa}\cdot\text{s}\cdot\text{m}^3\cdot\text{kg}^{-1}$.

The calibration of the oscillating-disk viscometer with argon and its error analysis were exemplified in ref 9 by one of the present authors (E. V.). The relative standard uncertainties of the reference viscosity value, $u_r(\eta_{0,\text{Ar,Vogel}}) = 0.0007$, as well as of the measuring quantities of the damped harmonic oscillation, that is, of the decrement, $u_r(\Delta) = 0.0005$, and of the period, $u_r(\tau) = 0.00005$, are to be considered to obtain the relative combined standard uncertainty of the Newell constant at room temperature, $u_{c,r}(C_N) = 0.0009$. To obtain the relative combined expanded ($k = 2$) uncertainty of the experimental viscosity data for water vapor, the relative standard uncertainties of C_N , of Δ , and of τ are to be taken into account. This leads to $U_{c,r}(\eta) = 0.002$ at room temperature and, assuming that the uncertainties could be slightly increasing with temperature, to $U_{c,r}(\eta) = 0.004$ at higher temperatures.

Teske et al.¹ performed additional measurements on argon between the measuring series on water vapor to detect any alterations in the suspension system of the viscometer due to possible reactions at higher temperatures between water vapor and quartz glass, of which the oscillating disk and the suspension wire are made of. Small changes in the Newell constant were taken into account by Teske et al. and in the present paper for the evaluation of the individual measuring series on water vapor. The re-evaluated results of the original series 1 to 10 and of the additional series A to D, including for each series two or three experimental data points at higher temperatures up to 497 or 527 K as well as two so-called remeasured experimental points at again lower temperatures, are given in Table S1 of the Supporting Information. The treatment of the re-evaluated data to receive η_0 viscosity values is described in detail in the Supporting Information. In addition, we have to take into account that some experimental points at low temperatures were measured at densities ρ higher than that of the saturated vapor, ρ_s . Thus, these experimental data correspond to the saturated vapor and the respective viscosity η_s given in Table S2 of the Supporting Information

for temperatures up to 339 K, was obtained by averaging them. Consequently, the number of re-evaluated data points that could be used to determine the η_0 value of an isotherm was reduced for the low-temperature isotherms. In particular, only three re-evaluated data points were available for the two isotherms close to 299 K, one of which resulted from measurements with increasing temperature and one from measurements with decreasing temperature (i.e., those performed after the highest temperature was attained). These circumstances required a separate procedure to infer the η_0 values, which is described in the Supporting Information. Moreover, only three experimental points were measured for the highest isotherm at 527 K.

2.2. Kinetic Theory Calculations. In the kinetic theory of polyatomic gases,³ the shear viscosity in the dilute-gas limit is given by

$$\eta_0(T) = \frac{k_B T}{\langle v \rangle} \frac{f_\eta^{(n)}}{S(2000)} \quad (1)$$

where $\langle v \rangle = 4(k_B T/\pi m)^{1/2}$ is the average relative thermal speed, k_B is Boltzmann's constant, m is the molecular mass, $S(2000)$ is a temperature-dependent generalized cross section, and $f_\eta^{(n)}$ is the n th-order correction factor.^{3,10} In this work, we evaluated $f_\eta^{(n)}$ up to $n = 3$ using the expressions given in ref 10. This requires 10 distinct cross sections for $f_\eta^{(2)}$ and 45 for $f_\eta^{(3)}$.

We calculated the required generalized cross sections by means of classical trajectories using an extended version of the TRAJECT software code.^{11,12} Trajectories describing collisions of two rigid H₂O molecules were obtained by integrating Hamilton's equations from pre- to postcollisional values, with the initial and final separation set to 100 nm. The CC-pol ab initio pair potential of Bukowski et al.^{13,14} was employed for these calculations. It was also used in our previous work on the transport properties of water vapor.² Of the four pair potentials tested in ref 2, CC-pol gave the best agreement with the available experimental data for shear viscosity. The CC-pol potential function was slightly modified as described in ref 2 to

avoid unphysical behavior at very small intermolecular separations. This modification does not have a negative impact on the accuracy of the calculated transport property values for the temperatures of interest in the present work.

Total-energy-dependent generalized cross sections, which are 13-dimensional integrals over the initial states of the trajectories, were computed for 25 values of the total energy (translational plus rotational) in the range from (160 to 50 000) K by means of a simple Monte Carlo procedure using quasirandom numbers. Up to 400 000 trajectories were computed for each total energy value. For energies below 1000 K, the number of trajectories had to be reduced because the computational demand required to calculate a trajectory with sufficient accuracy increases as the energy decreases. At 160 K, only 30 000 trajectories were calculated. However, the contributions of such low energies to the transport properties of water vapor for temperatures above 250 K are negligibly small. The final integration over total energy, which yields the temperature-dependent generalized cross sections, was performed using Chebyshev quadrature. Note that thermal conductivity values resulting from the present set of generalized cross sections have already been published.¹⁵

The calculated viscosity values reported by us in ref 2 are based on far fewer trajectories (only up to 80 000 for each total energy value). Moreover, they were calculated only up to the second-order approximation.

3. RESULTS AND DISCUSSION

The zero-density and initial-density viscosity coefficients η_0 and η_1 were obtained from fits of the re-evaluated viscosity data, converted to isotherms, using a series expansion in density truncated at first order

$$\eta(T, \rho) = \eta_0(T) + \eta_1(T)\rho \quad (2)$$

The values for η_0 and η_1 are presented in Table 1 together with their individual standard deviations σ_{η_0} and σ_{η_1} and with the standard deviation σ_η for each isotherm. A fit of the zero-density values of Table 1 (see eq S2 in the Supporting Information) shows that the deviations of the η_0 data of the measurements with increasing and decreasing temperature at about 299 K and 381 K from the fitted values are within ± 0.05 %. The consistency of the results for the measurements after attaining the highest temperature with those obtained before with increasing temperature reveals that any potential reactions between water vapor and quartz glass and subsequent alterations of the suspension system of the viscometer should be reversible.

Although the two η_0 values at room temperature nearly coincide, their quality is questionable because only three quasi-isothermal experimental data points at nearly the same densities, $0.018 < \rho/\text{kg}\cdot\text{m}^{-3} < 0.023$, could be used for the extrapolation to the limit of zero density. Therefore, the η_0 values at room temperature were additionally determined using the Rainwater–Friend theory^{16,17} to correct for the initial density dependence of the viscosity. These values are also given in Table 1.

Furthermore, Table 1 shows that the values of σ_η , σ_{η_0} , and σ_{η_1} of the fit of eq 2 to the quasiexperimental values for the isotherms 467 K, 497 K, and 527 K are considerably increased. Thus, the quality of the extrapolated values for the dilute-gas limit at higher temperatures is questionable. The most suitable way to test the reliability of the experimentally based η_0 values

at low as well as at high temperatures consists in a comparison with the theoretically calculated η_0 values.

The higher-order correction factors $f_\eta^{(2)}$ and $f_\eta^{(3)}$ in eq 1 are close to unity for all considered temperatures. For $f_\eta^{(2)}$, the results are similar to those of ref 2 with values between 1.0026 and 1.0055. For $f_\eta^{(3)}$, which was not considered in ref 2, we obtained, as expected, values close to those for $f_\eta^{(2)}$. The ratio $f_\eta^{(3)}/f_\eta^{(2)}$ varies between 0.9997 and 1.0002.

At temperatures around 300 K, we estimate that the relative standard uncertainties of the computed viscosity values due to the use of the rigid-rotor approximation, the neglect of quantum effects, uncertainties of the pair potential, the inaccuracy of the Monte Carlo integration, and the use of third-order kinetic theory are 0.5 %, 0.5 %, 0.5 %, 0.15 %, and 0.02 %, respectively, resulting in a relative combined expanded ($k = 2$) uncertainty of approximately 2 %. At far higher temperatures, the relative errors due to the use of the rigid-rotor approximation are probably larger, but the relative errors due to the neglect of quantum effects are certainly smaller. We therefore assume that our estimate for the relative combined expanded uncertainty at temperatures around 300 K is also valid for the whole temperature range from (250 to 2500) K. The computed viscosity values η_0 are given for selected temperatures in Table 2.

In Figures 1 and 2, we compare the computed viscosity values with the experimentally based re-evaluated data of the present work, the data reported by Teske et al.,¹ further

Table 2. Viscosity η_0 of Water Vapor in the Dilute-Gas Limit from Third-Order Kinetic Theory as a Function of Temperature T^a

T K	η_0 $\mu\text{Pa}\cdot\text{s}$	T K	η_0 $\mu\text{Pa}\cdot\text{s}$	T K	η_0 $\mu\text{Pa}\cdot\text{s}$
250.00	8.054	490.00	16.83	1000.00	37.65
260.00	8.383	500.00	17.24	1050.00	39.52
270.00	8.714	520.00	18.05	1100.00	41.35
273.15	8.819	540.00	18.88	1150.00	43.13
280.00	9.048	560.00	19.71	1200.00	44.87
290.00	9.384	580.00	20.54	1250.00	46.58
298.15	9.660	600.00	21.38	1300.00	48.24
300.00	9.723	620.00	22.23	1350.00	49.87
310.00	10.07	640.00	23.07	1400.00	51.47
320.00	10.41	660.00	23.91	1450.00	53.04
330.00	10.76	680.00	24.76	1500.00	54.57
340.00	11.11	700.00	25.60	1550.00	56.08
350.00	11.47	720.00	26.44	1600.00	57.55
360.00	11.83	740.00	27.27	1650.00	59.01
370.00	12.19	760.00	28.10	1700.00	60.44
380.00	12.56	780.00	28.93	1750.00	61.85
390.00	12.93	800.00	29.76	1800.00	63.23
400.00	13.31	820.00	30.57	1850.00	64.60
410.00	13.69	840.00	31.38	1900.00	65.95
420.00	14.07	860.00	32.19	1950.00	67.28
430.00	14.45	880.00	32.99	2000.00	68.59
440.00	14.84	900.00	33.79	2100.00	71.17
450.00	15.23	920.00	34.57	2200.00	73.69
460.00	15.63	940.00	35.35	2300.00	76.17
470.00	16.03	960.00	36.13	2400.00	78.59
480.00	16.43	980.00	36.89	2500.00	80.98

^aThe relative combined expanded ($k = 2$) uncertainty $U_{c,r}$ is $U_{c,r}(\eta_0) = 0.02$.

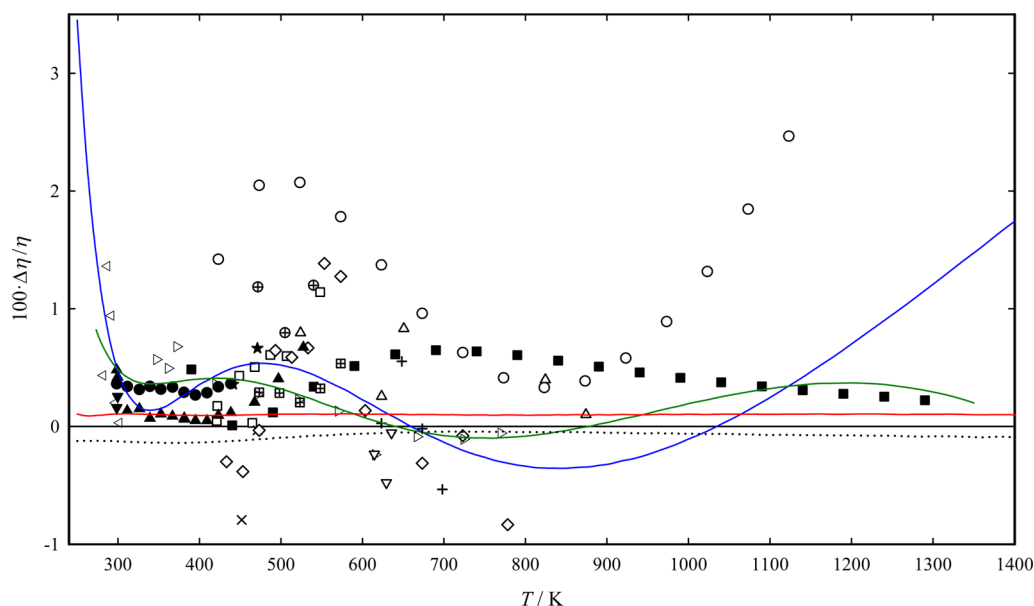


Figure 1. Relative deviations, $100 \cdot \Delta\eta/\eta = 100 \cdot (\eta_0 - \eta_{0,\text{calc}})/\eta_{0,\text{calc}}$ of experimental data, correlations, and theoretically calculated values for the viscosity of water vapor in the dilute-gas limit from values computed using third-order kinetic theory: \circ , Shifrin;¹⁸ \star , Kestin and Wang;¹⁹ \oplus , Moszynski;²⁰ \square , Kestin and Richardson;²¹ \blacksquare , Latto;²² \boxplus , Rivkin and Levin;²³ $+$, Rivkin et al.;²⁴ \times , Sato et al.;²⁵ \diamond , Sato et al.;²⁶ \triangleleft , Yasumoto;²⁷ \triangleright , Timrot et al.;²⁸ \triangle , Nagashima et al.;²⁹ ∇ , Oltermann;³⁰ \bullet , Teske et al.;¹ \blacktriangle , this work, obtained from extrapolation of isotherms; \blacktriangledown , this work, obtained from Rainwater–Friend theory; green line, correlation of Teske et al.;¹ blue line, IAPWS 2008 correlation;^{33,34} red line, correlation of this work (eq 3); dotted line, theoretically calculated values of Hellmann et al.²

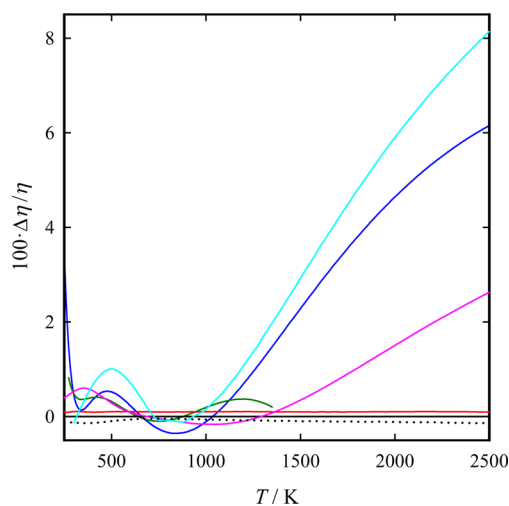


Figure 2. Relative deviations, $100 \cdot \Delta\eta/\eta = 100 \cdot (\eta_0 - \eta_{0,\text{calc}})/\eta_{0,\text{calc}}$ of correlations and theoretically calculated values for the viscosity of water vapor in the dilute-gas limit from values computed using third-order kinetic theory: purple line, correlation of Aleksandrov and Matveev;³¹ cyan line, correlation of Fokin and Kalashnikov;³² green line, correlation of Teske et al.;¹ blue line, IAPWS 2008 correlation;^{33,34} red line, correlation of this work (eq 3); dotted line, theoretically calculated values of Hellmann et al.²

experimental data from the literature,^{18–30} correlations,^{1,31–34} and the computed values of ref 2. Figure 1 illustrates that in the temperature range $311 \leq T/\text{K} \leq 438$ the present extrapolated η_0 data are approximately 0.1 % higher than the computed values of this work. The η_0 data at about 299 K corrected to the limit of zero density by means of the Rainwater–Friend theory differ by about +0.2 %, whereas the extrapolated η_0 data at this temperature deviate by +(0.4 to 0.5) %. In addition, the extrapolated η_0 data at the higher temperatures 467 K and 497

K and particularly at 527 K are characterized by increasing positive deviations up to +0.7 %. Therefore, the comparison of the temperature dependencies of the experimentally based data and of the computed values of the present work enables in fact to conclude that the reliability of the extrapolated values at 299 K and at the highest temperatures is distinctly reduced. On the basis of the observed deviations, a realistic estimate for the relative combined expanded ($k = 2$) uncertainty of all experimental data at the three highest temperatures is $U_{\text{cr}}(\eta) = 0.01$. The data reported by Teske et al.¹ are increased by another 0.2 % compared to the computed values due to the calibration with the out-of-date reference viscosity value for argon recommended by Kestin et al.⁴ The experimental data^{18–30} included in the comparison in Figure 1 are characterized by deviations between −0.9 % and +2.5 %. It is worth noting that the experimental data of Latto²² agree perfectly with the present computed values up to 1290 K; they differ by no more than +0.7 %. In contrast, the data of Shifrin¹⁸ are characterized by deviations of up to +2.5 % at 1123 K. Figures 1 and 2 clearly show that Shifrin’s data have strongly influenced the high-temperature extrapolation behavior of the correlation of Fokin and Kalashnikov³² and of the IAPWS 2008 correlation^{33,34} (which is valid for $273 \leq T/\text{K} \leq 1173$, with relative combined expanded ($k = 2$) uncertainties of 2 % below 773 K and 3 % above 773 K), resulting in deviations from the calculated values at 2500 K of +8.1 % and +6.2 %, respectively. The correlation of Aleksandrov and Matveev³¹ shows better high-temperature behavior with a deviation of +2.6 % at 2500 K, whereas the correlation of Teske et al.¹ is not intended for extrapolation to temperatures higher than 1350 K, where it deviates by just +0.2 %. The IAPWS 2008 correlation differs substantially from the calculated values also at very low temperatures with deviations increasing from only +0.1 % at 340 K to +3.5 % at 250 K. The calculated values reported by us

in ref 2 differ on average by -0.1% from the current calculated values.

As the comparison with the experimental data indicates that the viscosity values obtained using kinetic theory have the correct temperature dependence (i.e., the relative deviations from the true viscosity values should be nearly constant) and are too low by only about 0.1% , we propose to scale the kinetic theory values for η_0 by a factor of 1.001 for all temperatures to obtain reference values.

We fitted the parameters of the following function to the scaled viscosity values:

$$\frac{\eta_0}{\mu\text{Pa}\cdot\text{s}} = \frac{\sqrt{\bar{T}}}{\sum_{i=0}^7 a_i \bar{T}^{-i/2}} \quad (3)$$

where $\bar{T} = T/T_c$ with the critical temperature $T_c = 647.096\text{ K}$. The values of the coefficients a_i are given in Table 3. Relative

Table 3. Coefficients of the Proposed Dilute-Gas Viscosity Correlation (eq 3)

i	a_i
0	3.933738×10^{-2}
1	-2.361739×10^{-1}
2	1.059696
3	-2.300709
4	2.786190
5	-1.852813
6	6.352538×10^{-1}
7	-8.803352×10^{-2}

deviations between the scaled viscosity values and values resulting from eq 3 are within $\pm 0.01\%$ for all temperatures. The new correlation is also depicted in Figures 1 and 2. The relative combined expanded ($k = 2$) uncertainty of the correlation is estimated to be 0.4% between (300 and 500) K, which corresponds to the expanded uncertainty of most of the re-evaluated data of Teske et al.¹ It increases linearly with decreasing temperature between (250 and 300) K to 0.8% at 250 K and with increasing temperature between (500 and 2500) K to 2.0% at 2500 K. Note that our uncertainty estimate does not take into account the effect of dissociation at high temperatures.

4. CONCLUSIONS

The temperature dependencies of the re-evaluated experimental data by Teske et al.¹ and of the theoretically computed values of the present work agree excellently at temperatures between (311 and 438) K. The experimental data extrapolated to the zero-density limit differ only by about $+0.1\%$ from the calculated values, although this nearly exact match is most likely fortuitous. In contrast, the experimentally based values at 299 K and at the higher temperatures up to 527 K are affected by an uncertain extrapolation and by experimental problems due to reversible reactions between water vapor and quartz glass, respectively. At 299 K, the deviations from the calculated values could be reduced significantly by using the Rainwater–Friend theory^{16,17} for the initial density dependence instead of extrapolating the data. The proposed correlation for the zero-density limit in the temperature range from (250 to 2500) K, which is based on both the experimental data and the theoretically calculated values, represents a significant improve-

ment over the zero-density contribution of the current IAPWS viscosity correlation.^{33,34}

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jced.5b00599.

Experimental viscosity data for water vapor from 14 isochoric series of measurements with the oscillating-disk viscometer and detailed description of the procedures applied to determine η_0 , η_1 , and η_s viscosity values from these data. (PDF)

■ AUTHOR INFORMATION

Corresponding Author

*E-mail: robert.hellmann@uni-rostock.de. Phone: +49-381-4986509. Fax: +49-381-4986502.

Notes

The authors declare no competing financial interest.

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■ REFERENCES

- (1) Teske, V.; Vogel, E.; Bich, E. Viscosity measurements on water vapor and their evaluation. *J. Chem. Eng. Data* **2005**, *50*, 2082–2087.
- (2) Hellmann, R.; Bich, E.; Vogel, E.; Dickinson, A. S.; Vesovic, V. Calculation of the transport and relaxation properties of dilute water vapor. *J. Chem. Phys.* **2009**, *131*, 014303.
- (3) McCourt, F. R. W.; Beenakker, J. J. M.; Köhler, W. E.; Kušcer, I. *Nonequilibrium Phenomena in Polyatomic Gases*; Clarendon Press: Oxford, 1990; Vol. I: Dilute Gases.
- (4) Kestin, J.; Ro, S. T.; Wakeham, W. A. Viscosity of the noble gases in the temperature range 25–700°C. *J. Chem. Phys.* **1972**, *56*, 4119–4124.
- (5) Newell, G. F. Theory of oscillation type viscometers V: Disk oscillating between fixed plates. *Z. Angew. Math. Phys.* **1959**, *10*, 160–174.
- (6) Vogel, E.; Jäger, B.; Hellmann, R.; Bich, E. Ab initio pair potential energy curve for the argon atom pair and thermophysical properties for the dilute argon gas. II. Thermophysical properties for low-density argon. *Mol. Phys.* **2010**, *108*, 3335–3352.
- (7) Jäger, B.; Hellmann, R.; Bich, E.; Vogel, E. Ab initio pair potential energy curve for the argon atom pair and thermophysical properties of the dilute argon gas. I. Argon-argon interatomic potential and rovibrational spectra. *Mol. Phys.* **2009**, *107*, 2181–2188. Corrigendum: **2010**, *108*, 105.
- (8) Bich, E.; Mehl, J. B.; Hellmann, R.; Vesovic, V. In *Experimental Thermodynamics Vol. IX: Advances in Transport Properties of Fluids*; Assael, M. J., Goodwin, A. R. H., Vesovic, V., Wakeham, W. A., Eds.; The Royal Society of Chemistry: Cambridge, 2014; Chapter 7, pp 226–252.
- (9) Vogel, E. Reference viscosity of argon at low density in the temperature range from 290 K to 680 K. *Int. J. Thermophys.* **2010**, *31*, 447–461.
- (10) Hellmann, R. Ab initio potential energy surface for the carbon dioxide molecule pair and thermophysical properties of dilute carbon dioxide gas. *Chem. Phys. Lett.* **2014**, *613*, 133–138.
- (11) Heck, E. L.; Dickinson, A. S. Transport and relaxation cross-sections for pure gases of linear molecules. *Comput. Phys. Commun.* **1996**, *95*, 190–220.
- (12) Dickinson, A. S.; Hellmann, R.; Bich, E.; Vogel, E. Transport properties of asymmetric-top molecules. *Phys. Chem. Chem. Phys.* **2007**, *9*, 2836–2843.

- (13) Bukowski, R.; Szalewicz, K.; Groenenboom, G. C.; van der Avoird, A. Predictions of the Properties of Water from First Principles. *Science* **2007**, *315*, 1249–1252.
- (14) Bukowski, R.; Szalewicz, K.; Groenenboom, G. C.; van der Avoird, A. Polarizable interaction potential for water from coupled cluster calculations. I. Analysis of dimer potential energy surface. *J. Chem. Phys.* **2008**, *128*, 094313.
- (15) Hellmann, R.; Bich, E. An improved kinetic theory approach for calculating the thermal conductivity of polyatomic gases. *Mol. Phys.* **2015**, *113*, 176–183.
- (16) Friend, D. G.; Rainwater, J. C. Transport properties of a moderately dense gas. *Chem. Phys. Lett.* **1984**, *107*, 590–594.
- (17) Rainwater, J. C.; Friend, D. G. Second viscosity and thermal-conductivity virial coefficients of gases: Extension to low reduced temperature. *Phys. Rev. A: At., Mol., Opt. Phys.* **1987**, *36*, 4062–4066.
- (18) Shifrin, A. S. Viscosity of steam at atmospheric pressure. *Teploenergetika* **1959**, *6* (9), 22–27.
- (19) Kestin, J.; Wang, H. E. The viscosity of superheated steam up to 270 °C. *Physica* **1960**, *26*, 575–584.
- (20) Moszynski, J. R. The viscosity of steam and water at moderate pressures and temperatures. *J. Heat Transfer* **1961**, *83*, 111–122.
- (21) Kestin, J.; Richardson, P. D. The viscosity of superheated steam up to 275 °C: A refined determination. *J. Heat Transfer* **1963**, *85*, 295–301.
- (22) Latto, B. Viscosity of steam at atmospheric pressure. *Int. J. Heat Mass Transfer* **1965**, *8*, 689–720.
- (23) Rivkin, S. L.; Levin, A. Y. Experimental study of the viscosity of water and steam. *Teploenergetika* **1966**, *13* (4), 79–82.
- (24) Rivkin, S. L.; Levin, A. Y.; Izrailevskii, L. B. Experimental study of the viscosity of steam at temperatures up to 450 °C and pressures up to 350 bar. *Teploenergetika* **1968**, *15* (12), 74–78.
- (25) Sato, T.; Minamiyama, T.; Yata, J.; Oka, T. Measurement of viscosity of steam at moderate temperatures and pressures. *7th International Conference on Properties of Steam (ICPS)*; Tokyo, **1968**; Paper B-5.
- (26) Sato, T.; Minamiyama, T.; Yata, J.; Oka, T. A study of viscosity for steam at moderate pressures. *Proc. 45th Annu. Meet., Kansai Div. JSME* **1970**, *704*, 7–9.
- (27) Yasumoto, I. Viscosity of water vapor in the temperature range from 6 to 29 °C. *Bull. Chem. Soc. Jpn.* **1970**, *43*, 3917–3919.
- (28) Timrot, D. L.; Serednitskaya, M. A.; Besspalov, M. S. Experimental study of the viscosity of water vapor at temperatures from 50 to 500 °C and pressures from 0.06 to 1.5 bar. *Teploenergetika* **1973**, *20* (8), 78–80.
- (29) Nagashima, A.; Tanishita, I.; Murai, Y. Measurement of pressure effect on viscosity of steam. *J. Chem. Eng. Data* **1974**, *19*, 212–213.
- (30) Oltermann, G. Measurement of the viscosity of steam near the critical point. Ph.D. Thesis, Technische Universität Hannover, 1977.
- (31) Aleksandrov, A. A.; Matveev, A. B. Equation for the coefficient of dynamic viscosity in the region of existence of liquid and gaseous phases of water: Validation of the selected form of the equation. *Teplofiz. Vys. Temp.* **1998**, *36*, 719–724.
- (32) Fokin, L. R.; Kalashnikov, A. N. Reference data on the viscosity of rarefied steam at a temperature of 2000 to 2500 K. *High Temp.* **2000**, *38*, 224–230.
- (33) IAPWS. Release on the IAPWS formulation 2008 for the viscosity of ordinary water substance. International Association for the Properties of Water and Steam, 2008. www.iapws.org.
- (34) Huber, M. L.; Perkins, R. A.; Laesecke, A.; Friend, D. G.; Sengers, J. V.; Assael, M. J.; Metaxa, I. N.; Vogel, E.; Marš, R.; Miyagawa, K. New international formulation for the viscosity of H₂O. *J. Phys. Chem. Ref. Data* **2009**, *38*, 101–125.