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Erratum: "Wide-Ranging Reference Correlations for Dilute Gas Transport Properties Based on *Ab Initio* Calculations and Viscosity Ratio Measurements" [J. Phys. Chem. Ref. Data 49, 013101 (2020)] **FREE**

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The authors regret that in the original published version of the manuscript, the claimed uncertainty values appearing in the Abstract, Sec. 4, and the Conclusions differed slightly from those shown in Table 10.

The statement in the Abstract should read “The new reference dilute gas viscosity correlations span temperature ranges from at least 150 K to 1200 K, with relative uncertainties up to 90% (methane) lower than the original *ab initio* results. For the noble gases, *ab initio* calculations for the Prandtl number are used to develop reference correlations for thermal conductivity ranging from at least 100 K to 5000 K, with relative uncertainties ranging from 0.05% (krypton) to 0.11% (xenon).”

In the last paragraph of Sec. 4 (p. 10), the sentence should read “Exceptions to this include the revised data from May *et al.*,¹ which have had their uncertainty reduced by factors of between 1.3 and 2.2 (or, equivalently, a fractional change of between 23% and 55%) and are up to 90% smaller than the uncertainties of the values

calculated with the corresponding *ab initio* pair potentials listed in Table 6.”

The statement in the Conclusions should read “For fluids other than helium, this approach reduces the uncertainty currently achievable via a direct *ab initio* calculation by up to 90%: between 200 K and 400 K, the relative uncertainties of the reference viscosity correlations range from about 0.05% for Kr and H₂ to about 0.3% for propane. New reference correlations for the dilute gas thermal conductivity of five noble gases were also developed, covering the temperature range at least (100–5000) K with relative uncertainties ranging from 0.05% for krypton to 0.11% for xenon.”

The authors also note that corrections are needed in the following places (note that reference numbers in this Erratum refer to the Reference list in this Erratum, not to the numbering in the original paper):

In the Introduction, Paragraph 3 (p. 2) should have “(84 K–10 000 K for argon²)” instead of “(83 K–10 000 K for argon²).”

In Sec. 3, Table 6 should be replaced:

TABLE 6. List of the authors, temperature ranges, and the relative uncertainties in the viscosity, $u_r(\eta)$, and thermal conductivity, $u_r(\lambda)$, calculated from the corresponding *ab initio* potential.

| Gas | Authors | Temperature range (K) | $10^2 u_r(\eta)$ | $10^2 u_r(\lambda)$ |
|----------|-------------------------------------|-----------------------|---------------------|---------------------|
| Helium | Cencek <i>et al.</i> ³ | 1–10 000 | 0.001 | 0.001 |
| Neon | Bich <i>et al.</i> ^{4,5} | 25–10 000 | 0.1 | 0.1 |
| Argon | Vogel <i>et al.</i> ² | 83.81–10 000 | 0.1 | 0.1 ^a |
| Krypton | Jäger <i>et al.</i> ⁶ | 70–5 000 | 0.13 | 0.13 |
| Xenon | Hellmann <i>et al.</i> ⁷ | 100–5 000 | 0.14 | 0.14 |
| Methane | Hellmann <i>et al.</i> ⁸ | 80–1 500 | 1 ^b | |
| Nitrogen | Hellmann ⁹ | 70–3 000 | 0.5 ^a | |
| Hydrogen | Mehl <i>et al.</i> ¹⁰ | 20–2 000 | 0.08 ^{a,c} | |
| | | | 1 ^{b,d} | |
| Ethane | Hellmann ¹¹ | 90–1 200 | 0.15 ^e | |
| | | | 0.5 ^f | |
| Propane | Hellmann ¹² | 150–1 200 | 1 ^g | |
| | | | 0.5 ^h | |

^aThe viscosity values calculated *ab initio* were re-scaled to match experimental results but no further uncertainty estimate was provided.¹³ The uncertainty value here is taken from the original paper.

^bThe uncertainty was not mentioned in the publication and was estimated in this work based on comparisons with experimental measurements and other theoretical calculations.

^cFor 200 K < T < 400 K.

^dFor other temperatures.

^eFor 250 K < T < 700 K.

^fFor other temperatures.

^gFor 150 K < T < 250 K and 700 K < T < 1200 K.

^hFor 250 K < T < 700 K.

In Sec. 5, the first line should read “Deviation statistics between literature data from 70 sources and the reference equations developed in this work are shown in Table 11.”

For some of the literature sources, the claimed uncertainties or the transport property values were cited incorrectly. Table 11 should read as follows:

TABLE 11. Summary of literature sources for experimental dilute gas transport properties.^a

| Authors | Uncertainty (%) ^b | T (K) | N^c,d | RMS (%) | Bias (%) |
|------------------------------------|------------------------------|---------------|---------|---------|----------|
| Viscosities | | | | | |
| Helium | | | | | |
| Berg ^{14,15} | 0.035 | 298.15 | 1 | 0.08 | 0.08 |
| Clarke and Smith ¹⁶ | 1.0 | 77.45–373.90 | 10 | 0.70 | 0.62 |
| Dawe and Smith ¹⁷ | 1.0 | 293.2–1600 | 15 | 1.44 | –1.12 |
| Gough <i>et al.</i> ¹⁸ | 1.0 | 120–320 | 11 | 0.70 | 0.56 |
| Kestin <i>et al.</i> ¹⁹ | 0.2 | 328.15–678.15 | 7 | 0.33 | 0.30 |
| Kestin <i>et al.</i> ²⁰ | 0.3 | 298.15–778.15 | 9 | 0.44 | 0.41 |
| Maitland and Smith ²¹ | 1.5 | 295–1533 | 11 | 1.52 | –0.87 |
| Seibt <i>et al.</i> ²² | 0.30 | 293.15 | 1 | 0.29 | –0.29 |
| Tanaka <i>et al.</i> ²³ | 1.0 | 298.15–323.15 | 2 | 0.93 | 0.93 |
| Vogel <i>et al.</i> ²⁴ | 0.3 | 294.46–647.92 | 20 | 0.11 | 0.10 |
| Neon | | | | | |
| Clarke and Smith ¹⁶ | 1.0 | 77.45–373.90 | 10 | 0.75 | 0.66 |
| Dawe and Smith ¹⁷ | 1.0 | 293.2–1600 | 15 | 1.39 | –0.98 |
| Edwards ²⁵ | 1.0 | 194.75–717.65 | 6 | 1.04 | –0.82 |

TABLE 11. (Continued.)

| Authors | Uncertainty (%) ^b | T (K) | N ^{c,d} | RMS (%) | Bias (%) |
|--|--------------------------------------|---------------|------------------|---------|---------------------|
| Evers <i>et al.</i> ²⁶ | 0.15 | 298.15–348.15 | 2 | 0.06 | 0.03 |
| Johnston and Grilly ²⁷ | 0.5 | 80–300 | 27 | 1.00 | –0.88 |
| Trautz and Zimmermann ²⁸ | 0.4 | 90–523 | 13 | 1.55 | –1.42 |
| Argon | | | | | |
| Clarke and Smith ²⁹ | 0.5 | 114.35–374.60 | 12 | 0.38 | 0.32 |
| Dawe and Smith ¹⁷ | 1.0 | 293.2–1600 | 15 | 0.76 | –0.31 |
| Gough <i>et al.</i> ¹⁸ | 1.0 | 120–320 | 11 | 0.48 | 0.46 |
| Hurly <i>et al.</i> ³⁰ | 0.36 | 293.15–373.15 | 5 | 0.15 | 0.15 |
| Lin <i>et al.</i> ³¹ | 0.062 | 298.15–653.15 | 14 | 0.08 | –0.07 |
| Maitland and Smith ²¹ | 1.5 | 295–1533 | 11 | 0.61 | –0.067 |
| May <i>et al.</i> ¹ (this work) | 0.038 | 202.71–394.20 | 21 | 0.019 | –0.010 |
| Vogel ³² | 0.2 | 291.09–681.96 | 49 | 0.042 | –0.033 |
| Zhang <i>et al.</i> ³³ | 0.082 | 243.15–393.15 | 17 | 0.041 | –0.032 |
| Krypton | | | | | |
| Dawe and Smith ¹⁷ | 1.0 | 293.2–1600 | 15 | 0.81 | –0.29 |
| Gough <i>et al.</i> ¹⁸ | 1.0 | 120–320 | 11 | 0.48 | 0.47 |
| Humberg and Richter ³⁴ | 0.13 | 253.20–473.37 | 8 | 0.06 | –0.011 |
| Lin <i>et al.</i> ³⁵ | 0.10 | 243.15–393.15 | 16 | 0.05 | 0.03 |
| Maitland and Smith ²¹ | 1.5 | 295–1553 | 10 | 0.69 | –0.26 |
| Vogel ³⁶ | 0.1 ^e 0.2 ^f | 296.75–689.81 | 52 | 0.088 | –0.019 |
| Wilhelm and Vogel ³⁷ | 0.2 | 298.15–348.15 | 2 | 0.22 | 0.22 |
| Xenon | | | | | |
| Clarke and Smith ²⁹ | 0.5 | 176.0–374.6 | 9 | 0.33 | 0.28 |
| Dawe and Smith ¹⁷ | 1.0 | 293.2–1600 | 15 | 0.68 | 0.07 |
| Lin <i>et al.</i> ³⁵ | 0.11 | 303.15–393.15 | 9 | 0.06 | 0.05 |
| May <i>et al.</i> ¹ (this work) | 0.084 | 202.88–298.15 | 7 | 0.014 | -8×10^{-5} |
| Rigby and Smith ³⁸ | 1.0 | 293–972 | 14 | 1.38 | –1.08 |
| Vogel ³⁶ | 0.1 ^g 0.2 ^h | 295.04–649.53 | 20 | 0.085 | 0.013 |
| Methane | | | | | |
| Dawe <i>et al.</i> ³⁹ | 1.0 | 293–1050 | 9 | 0.57 | 0.29 |
| Gough <i>et al.</i> ¹⁸ | 1.0 | 150–320 | 10 | 0.62 | 0.61 |
| Humberg <i>et al.</i> ⁴⁰ | 0.25 | 253.16–473.17 | 9 | 0.09 | –0.058 |
| May <i>et al.</i> ¹ (this work) | 0.067 | 210.76–391.55 | 13 | 0.050 | 0.011 |
| Meerlender and Aziz ⁴¹ | 1.0 | 293.15–353.15 | 6 | 0.39 | –0.36 |
| Schley <i>et al.</i> ⁴² | 0.3 | 260–360 | 6 | 0.036 | 0.020 |
| Vogel ⁴³ | 0.2 | 289.05–682.14 | 35 | 0.21 | 0.20 |
| Hydrogen | | | | | |
| Barua <i>et al.</i> ⁴⁴ | 0.22 | 223.15–423.15 | 6 | 0.42 | –0.23 |
| Gracki ⁴⁵ | 0.11 | 173.15–298.15 | 3 | 0.44 | –0.41 |
| Hongo and Iwasaki ⁴⁶ | 0.3 | 298.15–373.15 | 4 | 0.39 | –0.026 |
| May <i>et al.</i> ¹ (this work) | 0.055 | 213.62–394.21 | 15 | 0.016 | 0.014 |
| Van Cleave and Maass ⁴⁷ | 1.0 | 89.75–295.15 | 2 | 0.54 | –0.54 |

TABLE 11. (Continued.)

| Authors | Uncertainty (%) ^b | T (K) | N ^{c,d} | RMS (%) | Bias (%) |
|--|------------------------------|---------------|------------------|---------|----------|
| Nitrogen | | | | | |
| El Hawary ⁴⁸ | 0.25 | 253.16–473.17 | 7 | 0.52 | 0.47 |
| Hoogland <i>et al.</i> ⁴⁹ | 0.1 | 298.11–333.10 | 5 | 0.11 | 0.098 |
| Humberg <i>et al.</i> ⁵⁰ | 0.10 | 253.21–473.38 | 9 | 0.066 | –0.060 |
| Seibt <i>et al.</i> ⁵¹ | 0.3 | 298.15–423.15 | 4 | 0.099 | 0.086 |
| Seibt <i>et al.</i> ²² | 0.3 | 293.18–423.11 | 2 | 0.34 | –0.32 |
| Trautz and Baumann ⁵² | 1.0 | 195.15–523.25 | 19 | 1.08 | –0.70 |
| Vogel ⁵³ | 0.20 | 291.55–681.99 | 17 | 0.064 | 0.050 |
| Ethane | | | | | |
| Iwasaki and Takahashi ⁵⁴ | 0.3 | 298.15–348.15 | 8 | 0.19 | –0.13 |
| Wilhelm <i>et al.</i> ^{55,56} | 0.25 | 289.97–429.96 | 8 | 0.35 | –0.34 |
| Vogel <i>et al.</i> ^{57,58} | 0.3 | 289.83–675 | 19 | 0.054 | –0.022 |
| Propane | | | | | |
| Abe <i>et al.</i> ⁵⁹ | 0.3 | 298.15–468.15 | 5 | 0.70 | 0.60 |
| Holland <i>et al.</i> ⁶⁰ | 1.0 | 160–500 | 18 | 0.77 | 0.48 |
| Kestin <i>et al.</i> ⁶¹ | 0.2 | 298.15–478.18 | 13 | 0.93 | 0.85 |
| Seibt <i>et al.</i> ⁶² | 0.3 | 273.18–366.10 | 3 | 0.93 | –0.58 |
| Vogel ⁶³ | 1.0 | 297.24–625.80 | 70 | 0.28 | 0.19 |
| Wilhelm and Vogel ^{64,65} | 0.25 | 298.21–423.09 | 7 | 0.24 | –0.19 |
| Thermal conductivities | | | | | |
| Helium | | | | | |
| Assael <i>et al.</i> ⁶⁶ | 0.2 | 308.15 | 1 | 0.08 | –0.08 |
| Baker ⁶⁷ | 0.5 | 300–600 | 8 | 0.21 | –0.06 |
| Kestin <i>et al.</i> ⁶⁸ | 0.3 | 300.65 | 1 | 0.55 | 0.55 |
| Mukhopadhyay and Barua ⁶⁹ | 1.0 | 90.18–473.25 | 6 | 0.52 | –0.38 |
| Mustafa <i>et al.</i> ⁷⁰ | 0.5 | 308.11–425.44 | 4 | 1.41 | 1.38 |
| Neon | | | | | |
| De Groot <i>et al.</i> ⁷¹ | 1.5 | 301.16 | 1 | 1.38 | –1.38 |
| Kestin <i>et al.</i> ⁶⁸ | 0.3 | 300.65 | 2 | 0.020 | 0.017 |
| Keyes ⁷² | 2.0 | 91.05–273.15 | 5 | 1.19 | –1.17 |
| Sengers <i>et al.</i> ⁷³ | 1.0 | 298.15–348.15 | 5 | 0.62 | –0.60 |
| Sevast'yanov and Zykov ⁷⁴ | 2.0 | 100–600 | 12 | 0.78 | –0.67 |
| Argon | | | | | |
| Assael <i>et al.</i> ⁶⁶ | 0.2 | 308.15 | 1 | 0.32 | 0.32 |
| Haran <i>et al.</i> ⁷⁵ | 0.3 | 308.15–429.15 | 5 | 0.63 | 0.42 |
| May <i>et al.</i> ¹ (this work) | 0.038 | 202.71–394.20 | 21 | 0.017 | –0.009 |
| Millat <i>et al.</i> ⁷⁶ | 0.3 | 308.15–428.15 | 4 | 0.77 | 0.69 |
| Roder <i>et al.</i> ⁷⁷ | 0.5 | 300.81–340.87 | 48 | 0.46 | –0.08 |
| Sun <i>et al.</i> ⁷⁸ | 1.0 | 296.84–427.80 | 36 | 0.39 | –0.009 |
| Krypton | | | | | |
| Assael <i>et al.</i> ⁶⁶ | 0.2 | 308.15 | 1 | 0.17 | 0.17 |
| Vargafik ⁷⁹ | 2.0 | 125–700 | 13 | 1.80 | 1.53 |
| Voshchinin <i>et al.</i> ⁸⁰ | 2.0 | 591–976 | 7 | 1.78 | 1.27 |

TABLE 11. (Continued.)

| Authors | Uncertainty (%) ^b | T (K) | N ^{c,d} | RMS (%) | Bias (%) |
|--|------------------------------|---------------|------------------|---------|--------------------|
| Xenon | | | | | |
| Assael <i>et al.</i> ⁶⁶ | 0.20 | 308.15 | 1 | 0.23 | 0.23 |
| Keyes ⁸¹ | NA | 214.25–273.15 | 7 | 0.42 | 0.10 |
| May <i>et al.</i> ¹ (this work) | 0.084 | 202.88–298.15 | 7 | 0.014 | 2×10^{-4} |
| Springer and Wingeier ⁸² | 1.0 | 900–2500 | 9 | 0.70 | –0.54 |

^aLiterature data measured at low pressures were also included and were corrected to the dilute gas condition via Rainwater and Friend theory.⁸³

^bThe reported uncertainties sometimes change with temperature slightly. Under these circumstances, the largest uncertainty is given in the table.

^cSome isothermal transport property data were reported at various pressures. In this case, only the lowest pressure point was corrected to the dilute gas condition for comparison.

^dThe N value only includes the points fitted in this work. Data that are inconsistent with other reported measurements were not included.

^eFor 295 K < T < 400 K.

^fFor 400 K < T < 690 K.

^gFor 295 K < T < 400 K.

^hFor 400 K < T < 650 K.

Some of the corrections in Table 11 affect the magnitude of the deviation for a given data point, the size of uncertainty bars, and the captions of Figs. 6–14. However, these have no significant impact on the deviation plots shown.

The authors would like to apologize for any inconvenience caused. Fortunately, these minor errors have no impact on the primary conclusions of the paper.

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