Wide-Ranging Reference Correlations for Dilute Gas Transport Properties Based on Ab Initio Calculations and Viscosity Ratio Measurements

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Reference correlations for dilute gas properties are important for apparatus calibration and predicting property values at extreme conditions. Ab initio calculations of dilute gas properties are rapidly improving in terms of both the number of substances described and the uncertainty with which they can be calculated. Such calculations have advantages over experiments in terms of the range of conditions that can be covered. However, with the exception of helium, dilute gas transport properties measured around ambient temperature have smaller uncertainties than theoretically-derived values. In 2007, May et al. reported an experimental method for transferring the very small uncertainty achieved in ab initio calculations for helium to other gases over a temperature range of 200 to 400 K. Subsequently, Berg and Moldover reported reference viscosity ratios for eleven gases relative to helium based on an analysis of multiple experimental studies. In parallel, significant theoretical progress has been made, both for helium via the work of Cencek et al. in 2012, and for other gases through the development of improved ab initio potentials that allow robust estimates of their transport properties with uncertainties of just a few percent over a wide temperature range. Here we extend the results obtained by May et al. to wider temperature ranges and to more gases. Ratios of transport properties calculated ab initio for a single gas at two different temperatures have a significantly lower uncertainty than that of the absolute values. By combining these calculated ratios with the reference experimental viscosity ratios determined by Berg and Moldover and with the reference helium viscosities calculated by Cencek et al., the accuracy achievable for helium can be transferred to many other gases at temperatures ranging between 100 and 1000 K. Estimates of the resulting uncertainty are presented, and noble gas thermal conductivities are also considered.