

Ab Initio Kinetic Coefficients of Gaseous Hydrogen

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The spherical portion of the hydrogen intermolecular potential recently determined in *ab initio* calculations by Patkowski *et al* [J. Chem. Phys. 129:094304 (2008)] was used to calculate the viscosity and spherical contribution to the thermal conductivity of hydrogen using a full quantum-mechanical formalism. Viscosities in the temperature range 203 K–394 K were compared with recent high-accuracy (uncertainty of 0.084 %) measurements of May *et al* [Int. J. Thermophys. 28:1085 (2007)]. The measured viscosities all fall in a range between 0.01 % and 0.06 % below the calculated viscosities. This close agreement supports the accuracy of the potential of Patkowski *et al*. The thermal conductivity, calculated in the modified Eucken approximation using literature values of the specific heat, was found in reasonable agreement with experimental results. The average fractional difference between three experimental data sets for hydrogen spanning 21–314 K was $(0.3 \pm 1.0) \%$; the average fractional difference between three experimental data sets for parahydrogen spanning 20–275 K was $(-0.8 \pm 1.2) \%$.