Ab Initio Potential Energy Curve for the Argon Atom Pair and Thermophysical Properties of the Dilute Argon Gas

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Argon is an important model substance for the development of simulation techniques. Hence, accurate potential energy curves are needed to describe the interactions between two argon atoms. One strategy to obtain pair potentials is to fit a function to experimental data of thermophysical properties such as the second pressure virial coefficient and zero-density viscosity. Since these properties can be determined with high precision only in limited temperature ranges, the resulting empirical potentials are restricted with regard to their reliability. Recently, we have demonstrated for helium and neon that potential functions completely calculated from theory lead to highly accurate values for thermophysical properties of the dilute gas. Interaction energies have been computed for 38 interatomic argon-argon distances at the CCSD(T) level of theory with the best available basis sets. Counterpoise correction, frozen-core approximation and extrapolation of the correlation energy to the complete basis set limit have been applied. Furthermore, corrections for core-core and core-valence correlation, for relativistic effects and for the impact of higher coupled-cluster terms (CCSDT,CCSDT(Q)) have been included. An analytical potential function of the HFD-ID type has been fitted to the resulting interaction energies. Eventually, the classical second and third pressure virial coefficients including quantum corrections and non-additive three-body contributions have been calculated. Since comparison with transport properties in the limit of zero density enables further stringent tests of the potential function, the viscosity and thermal conductivity coefficients of the dilute gas have been determined by means of the kinetic theory. All results show excellent agreement with the best experimental data in restricted temperature ranges. At very low and high temperatures, the theoretical values are more reliable than the experiments. The findings demonstrate a considerable improvement of the new potential compared to other *ab initio* potentials from the literature.