

Calculations of Thermophysical Properties of Gaseous Neon-Argon Mixtures from State-Of-The-Art *Ab Initio* Pair Potentials

Eckard Bich^{C,S}, Robert Hellmann, Benjamin Jäger and Eckhard Vogel
Institute of Chemistry, University of Rostock, Rostock, Mecklenburg-Vorpommern, Germany

The binary mixture neon-argon represents a model system which can be used for the calibration of measuring instruments for diffusion and thermal diffusion. For that purpose highly accurate values of the transport properties as well as of the second and third pressure virial coefficients can be calculated from the kinetic theory of gases and statistical thermodynamics. Prerequisite for that are accurate potential energy curves for all pairwise interactions between the atoms in the mixture. The *ab initio* potential functions for helium and neon were computed in our group and used to derive highly accurate values for thermophysical properties of these gases. Now we have calculated the interatomic potentials for neon-argon and argon-argon so that all three pair potentials needed for the mixtures of neon and argon are now available. Interaction energies for all three potentials have been computed for a large number of interatomic 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. Analytical potential functions of the HFD-ID type have been fitted to the resulting interaction energies of each pair of atoms. The classical second and third pressure virial coefficients including quantum corrections, the binary and thermal diffusion coefficients as well as the viscosity and thermal conductivity coefficients were determined and compared with experimental data. All results show close agreement with the best experimental data in restricted temperature ranges. The theoretical values are generally more reliable than the experiments at all temperatures relevant for practical purposes.