Thermophysical Property Predictions for Gaseous Methane-Nitrogen and Propane-Helium Mixtures from *Ab Initio* Potential Energy Surfaces

Benjamin Jäger [C, S], Robert Hellmann and Eckard Bich
Institut für Chemie, Universität Rostock, Rostock, Germany
benjamin.jaeger@uni-rostock.de

In recent years, quantum-chemical methods have become a valuable tool for the development of highly accurate interaction potentials for atoms and small molecules. Such potentials can be used to compute reference values for thermophysical properties of pure gases and gaseous mixtures for large temperature ranges by means of the kinetic theory of dilute gases and of statistical thermodynamics. Interaction energies obtained from high-level *ab initio* coupled-cluster methods were used to develop accurate pair potential energy surfaces for the systems methane-nitrogen and propane-helium. We computed second interaction virial coefficients applying the Mayer-sampling Monte Carlo procedure [1] and compared the results with experimental data to verify the quality of the potentials. Furthermore, classical trajectory calculations were performed for all binary collisions involved in the dynamics of the gas mixtures under study. This included also the interaction potentials for the pure species [2-4]. The kinetic theory of dilute gases was employed to obtain the transport coefficients of the gas mixtures. We compare the theoretical results with the best experimental data for the viscosity, thermal conductivity and the binary and thermal diffusion coefficients.

References

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