

Transport Properties of Noble Gas and Ammonia-Helium Mixtures from *Ab Initio* Potentials Using a New Formulation of the Kinetic Theory of Gases

Benjamin Jäger^{C, S}, Robert Hellmann and Eckard Bich
University of Rostock, Institute of Chemistry, Rostock, Germany
benjamin.jaeger@uni-rostock.de

The accurate determination of thermophysical properties for binary mixtures of simple fluids can be regarded as model case for industrially relevant substances. Reliable data for mixtures with ammonia are of special interest in the field of refrigeration. Furthermore, the correct description of the intermolecular interactions in such systems is a challenging task from a theoretical point of view due to the intramolecular inversion behavior of the ammonia molecule. In times of growing computational resources it has become possible to develop interaction potentials for atoms and small molecules from pure theory, i.e. with the help of quantum-chemical *ab initio* methods. These potentials can be combined with statistical mechanics to obtain highly accurate thermophysical properties. New *ab initio* pair potential functions for the helium-krypton atom pair and for the ammonia-helium system will be presented. Moreover, a new generalized kinetic theory for dilute gaseous mixtures has been derived, which is applicable for approximations of arbitrary order and for any types of molecules. Transport properties in the zero-density limit have been calculated using the kinetic theory in the fifth-order approximation for neon-argon and helium-krypton mixtures. For these computations, highly reliable *ab initio* pair potentials for the pure substances [1-3] have been employed as well. The results are characterized by good agreement with the best experimental data and may serve as reference values. The transport coefficients of ammonia-helium mixtures will be presented for the second-order approximation of the kinetic theory. These results are regarded as a test for the extension of the kinetic theory of pure molecular gases to molecular gas mixtures.

- [1] R. Hellmann, E. Bich, E. Vogel, *Mol. Phys.* **105**, 3013 (2007).
- [2] R. Hellmann, E. Bich, E. Vogel, *Mol. Phys.* **106**, 133 (2008).
- [3] B. Jäger, R. Hellmann, E. Bich, E. Vogel, *Mol. Phys.* **108**, 105 (2010).