

Metrological Use of Thermophysical Properties of Gases from Ab Initio Calculations and Precision Experiments

Christof Gaiser^{1, S, C} and Bernd Fellmuth²

¹*PTB, Berlin, Germany*

²*PTB (retired), Berlin, Germany*
christof.gaiser@ptb.de

The development of ab initio calculations within the last two decades, especially in the field of noble gases, is very impressive. The achievements together with possible applications were recently summarized in [1]. Nowadays, the ab initio calculations of thermophysical properties, especially for helium, have smaller uncertainties than the most accurate experimental determinations. In the case of higher noble gases like neon and argon, for some quantities, precision experiments are still one step ahead [2]. The main applications of accurate data for thermophysical properties like polarizability and virial coefficients can be found in the field of thermometry and pressure metrology.

As an example, low-temperature thermometry using dielectric-constant gas thermometry (DCGT) [3] will be discussed. This primary thermometry method is part of the *Mise en Pratique* for the definition of the kelvin and, therefore, an allowed way of realizing the base unit kelvin. With improved thermophysical property data, different application variants of DCGT are now possible. A summary and the achievements for the three noble gases helium, neon, and argon will be shown.

A second example is an alternative pressure standard [4]. The latest improvements for helium [5,6] will be presented, showing that this method is a real alternative to a classical pressure standard. In addition, neon and argon as working gases for the pressure standard will be tested. In these cases, the input quantities stem from ab initio calculations as well as from precision experiments.

Finally, recent measurements of the polarizability of krypton will be presented. A possible use and the resulting advantages will be discussed.

References

1. G. Garberoglio, C. Gaiser, R. M. Gavioso, A. H. Harvey, R. Hellmann, B. Jeziorski, K. Meier, M. R. Moldover, L. Pitre, K. Szalewicz and R. Underwood, *J. Phys. Chem. Ref. Data* 52, 031502 (2023)
2. C. Gaiser and B. Fellmuth, *J. Chem. Phys.* 150, 134303 (2019)
3. C. Gaiser, B. Fellmuth and T. Zandt, *Metrologia* 52, S217 (2015)
4. M. R. Moldover, *J. Res. Natl. Inst. Stand. Technol.* 103, 167 (1998)
5. C. Gaiser, B. Fellmuth and W. Sabuga, *Nature Physics*, 16, 177 (2020)
6. C. Gaiser, B. Fellmuth and W. Sabuga, *Ann. Physik* 534, 2200336 (2022)