URN (Paper): urn:nbn:de:gbv:ilm1-2011iwk-013:1

56[TH] INTERNATIONAL SCIENTIFIC COLLOQUIUM
Ilmenau University of Technology, 12 – 16 September 2011
URN: urn:nbn:gbv:ilm1-2011iwk:5

NEW DEFINITION OF THE KELVIN AND DETERMINATION OF THE BOLTZMANN CONSTANT

Joachim Fischer and Thorsten Zandt

Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

ABSTRACT

The unit of temperature *T*, the kelvin is presently defined by the temperature of the triple point of water. Thus, the kelvin is linked to a material property. Instead, it would be advantageous to proceed in the same way as with other units: to relate the unit to a fundamental constant and fix its value. For the kelvin, the corresponding constant is the Boltzmann constant *k*, because temperature always appears as thermal energy *kT* in fundamental laws of physics. Many projects are under way to measure independently the value of the Boltzmann constant. These are acoustic gas thermometry measuring the speed of sound and dielectric-constant gas thermometry using audio-frequency capacitance bridges. Other promising methods are Doppler-broadening thermometry and Johnson noise thermometry. The progress achieved so far and the potential of the methods by the time of the redefinition will be reviewed.

Index Terms – fundamental constant, Boltzmann constant, temperature measurement, temperature scale, base units

1. INTRODUCTION

The International System of Units, the SI, is a coherent system of units for use throughout science and technology. The units of the SI provide the framework for measuring all the quantities that occur in the equations of the physical sciences. The equations among the quantities are independent of the way in which the units are defined. The values of all the fundamental constants are invariants of nature, but their numerical values depend on the units in which they are expressed. Fixing the numerical values of a set of constants defines a particular set of units, which is the SI. This also has the effect of fixing the numerical values of all other constants that can be written as products and ratios of these constants. It is important to note that for those constants whose numerical values have not been fixed, their values still remain invariants of nature, although their numerical values have to be determined by experiment.

The present definition of the unit of thermodynamic temperature was given in substance by the 10th General Conference on Weights and Measures in 1954, which selected the triple point of water, T_{TPW}, as a fundamental fixed point: The temperature unit kelvin is the 273.16th part of the thermodynamic temperature of the triple point of water. This definition derives the unit from a rather randomly selected material property. Thus, influences of the isotope composition and the purity of the used water are of essential importance for their practical realisation. Thereby, the stability of the realisation over space and time is jeopardised.

Since the establishment of the SI in 1960, extraordinary advances have been made in relating SI units to truly invariant quantities such as the fundamental constants of physics and the properties of atoms. Recognising the importance of linking SI units to such invariant quantities, the International Committee for Weights and Measures (CIPM) adopted in 2005 a recommendation to prepare for new definitions of the kilogram, ampere, kelvin, and mole in terms of fixed numerical values of the Planck constant, elementary charge, Boltzmann constant *k*, and Avogadro constant, respectively.

The CIPM recommended the national metrology institutes to submit adequate proposals for the kelvin - in the same way as for the kilogram, the ampere and the mole – to make sure that these four base units can be newly defined [1]. The aim is to define, in future, the base units via fundamental constants and to make them thus independent of embodied standards, so-called artefacts, or special measurement instructions. As the thermodynamic temperature *T* always occurs in the combination *kT* as "thermal energy" in all fundamental laws, the Boltzmann constant *k* is the natural constant to be fixed. By determining its value, the kelvin is directly derived from the unit of energy "the joule" (similar to the unit of length “meter” by determining the value of the speed of light of the unit of time "second" since 1983).

At present, it is not necessary to modify the structure of the International System of Units and to select other base units [2]. The kelvin should therefore not disappear from this system. A new definition should be of use both for daily application in development and production and for fundamental research. To avoid recalibrations and conversions, no verifiable discontinuity should occur in the quantity of the unit. The uncertainty of the value of the relevant fundamental constant should thus be comparable to the uncertainty of the realisation pursued so far.

The 2006 internationally accepted value [3] of $1.3806504 \cdot 10^{-23}$ J/K for the Boltzmann constant has a relative standard uncertainty of $1.7 \cdot 10^{-6}$. This value and its uncertainty are mainly based on a single measurement by means of acoustic gas thermometry at the United States National Institute of Standards and Technology (NIST) in the year 1988. However, one single measurement is not considered to be a sufficient base for fixing of the numerical value. Therefore, a concept was discussed at two workshops at PTB in Berlin with the experts of all important metrology institutes and a time schedule was elaborated in order to achieve a value of k which is based on several different methods [4]. In the following, the customary primary thermometer methods to determine k are presented, together with the achieved uncertainties and the uncertainties to be expected.

2. METHODS FOR THE DETERMINATION OF THE BOLTZMANN CONSTANT

As the mean microscopic thermal energy kT is not directly experimentally accessible, macroscopic quantities, which are clearly correlated with the thermal energy [5], must be measured for the determination of k at the triple point of water. Table 1 gives an overview over such dependencies in which T is only related to other *measurable* quantities and known constants. For ideal gases, the thermal energy is proportional to the mean kinetic energy of the gas particles. In a closed volume, this energy is measurable via the gas pressure and the number of particles. The pressure p is described for a negligible interaction between the particles by means of the equation of state of the ideal gas. The thermometer based on this law is the traditional gas thermometer whose uncertainty, however, is too large for absolute measurements. On the other hand, the density, which changes with the temperature at a constant pressure, can be determined via the dielectric constant or the refractive index. Also the speed of sound in a gas serves as a temperature indicator (acoustic gas thermometer).

If you use the conducting electrons of a metallic resistance as a "measuring substance", the electrical Johnson noise according to the Nyquist formula is suited for thermometry. Laser spectroscopy provides the kinetic energy of the absorbing atoms from the Doppler broadening of absorption lines. Table 1 also lists the uncertainties to be expected for the determination of k. A compact description of all current methods can be found in the overview article [5].

Table 1: Overview of the primary thermometers which are suitable for the determination of the Boltzmann constant k, with the relative uncertainties to be expected (T Temperature, u_0 speed of sound in the limiting case of disappearing pressure and of very low frequency, $\gamma_0 = c_p/c_V$ ratio of the specific heat, M molar mass of the gas,. R molar gas constant, p pressure, ε dielectric constant, ε_0 electric constant, α_0 static electrical polarizibility, n refractive index, $\langle U^2 \rangle$ mean square noise voltage, R_{el} electric resistance, ν frequency, $\Delta\nu_D$ Doppler width of a spectral line of the frequency ν_0, m atomic mass, c_0 speed of light in the vacuum).

Primary thermometric method	**Law of physics**	**Achievable relative standard uncertainty**
Acoustic gas thermometer	$u_0 = \sqrt{\frac{\gamma_0 RT}{M}}$	$1 \cdot 10^{-6}$
Dielectric constant gas thermometer	$p = kT\frac{(\varepsilon - \varepsilon_0)}{\alpha_0}$	$2 \cdot 10^{-6}$
Refractive index gas thermometer	$p = kT\frac{(n^2 - 1)\varepsilon_0}{\alpha_0}$	$10 \cdot 10^{-6}$
Johnson noise thermometer	$\langle U^2 \rangle = 4kTR_{el}\Delta\nu$	$5 \cdot 10^{-6}$
Doppler broadening thermometer	$\Delta\nu_D = \sqrt{\frac{2kT}{mc_0^2}}\nu_0$	$10 \cdot 10^{-6}$

2.1. Acoustic gas thermometer

In a gas, a number of measurands depend on temperature. As the describing equations are generally derived for ideal gases and the interaction between the gas particles for the determination of k is not sufficiently known, the measurements are carried out by means of extrapolation to zero pressure in such a way that the approximation of the ideal gas is sufficient. For the determination of k at NIST, the speed of sound u_0 of the noble gas argon was determined by means of a spherical resonator (Figure 1) at the temperature of the triple point of water and k was calculated from the respective formula in Table 1, whereby the molar gas constant R is replaced by kN_A (N_A Avogadro constant).

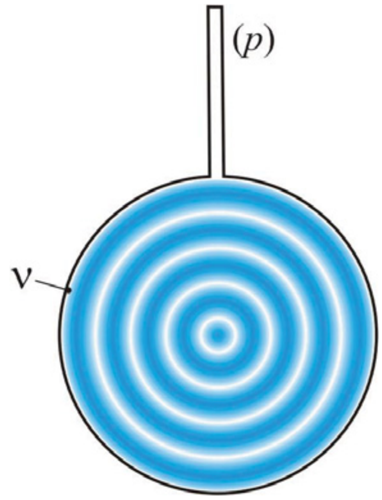

Figure 1: Principle of acoustic gas thermometer with spherical resonator. The sound velocity u_0 is derived from the resonance frequencies ν and the volume of the resonator. The influence of pressure p is only of second order.

Spherical resonators are also used at other institutes now [5]. The resonator dimensions were determined at NIST by a mercury filling of known density. Today, the resonator is measured by means of microwave resonances. Besides the determination of the dimensions and the connection to the triple point temperature, essential uncertainty contributions result from the dependency of the molar mass on the isotope composition, the purity of the measuring gas, the extrapolation to zero pressure and the position of the acoustic transducers. With the current measuring technique, an uncertainty of $1 \cdot 10^{-6}$ is attainable when using this method.

2.2. Dielectric constant gas thermometer

The determination of the dielectric constant of helium has been in use for a long time in thermometry for low temperatures and is - compared to the measurement of the refractive index - the more advanced and more promising procedure which offers far smaller attainable uncertainties. For an ideal gas, the dielectric constant is given by $\varepsilon = \varepsilon_0 + \alpha_0 \cdot N/V$ (N/V for the density of their number of particles). By combining it with the equation of state, the relation between p and ε indicated in Table 1 is obtained. Considerable progress made with the ab-initio calculation of the polarizibility of helium, whose uncertainty could be reduced to less than $1 \cdot 10^{-6}$ in the past few years, has made this method competitive. To measure ε, the measuring gas is filled into suitable capacitors. Due to the very low polarizibility of helium, absolute measurements are not possible. Therefore, the measuring capacitor is alternately filled with helium and evacuated, and ε is derived from the relative change in capacitance (Figure 2).

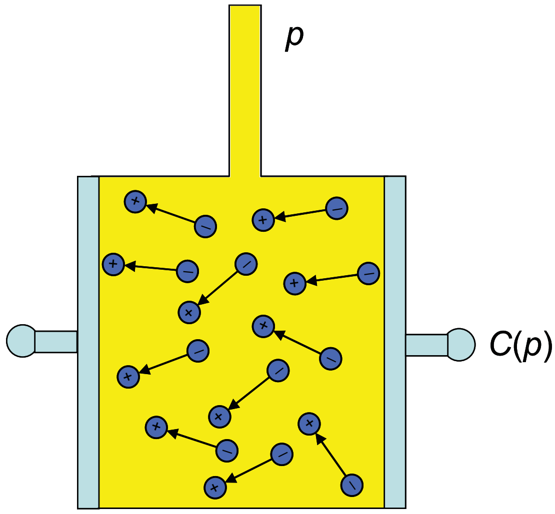

Figure 2: The central element of the dielectric constant gas thermometer is the measuring capacitor, which is filled with gas with the pressure p, and whose relative capacity change $(C(p)\text{-}C(0))/C(0)$ is measured.

A considerable source of error when using this method results from the deformation of the measuring capacitor due to the gas pressure. The pressure and capacitance measurements must also be improved to the best possible extent. The estimation of all contributions allows an overall uncertainty comparable to acoustic gas thermometry of about $2 \cdot 10^{-6}$ to be expected. This estimation is supported by the results which have recently been achieved in measurements in the low-temperature range from 2.5 K to 36 K [6] and at the TPW [7].

2.3. Johnson noise thermometer

The temperature of an object can also be determined by observing statistical or quantum effects. For many years, noise thermometry has been used in thermometry. Noise thermometry determines temperature - by means of the Nyquist formula (Table 1) - from the mean square of the noise voltage which drops at an electric resistance. The electric resistance value of the test sample at the triple point of water as well as the amplification and bandwidth of the electronic measuring system have to be determined precisely as parameters.

So far, noise thermometry has been well-established at very low and very high temperatures. At high temperatures, it uses the larger measurement signals and is thus less sensitive to disturbances. At low temperatures, highly sensitive, superconducting detectors can be used and the small signals can be evidenced by adequate signal-to-noise ratio. In the area around the triple point of water, particular electronic circuits, e.g. alternately switching digital correlator, have to be used and comparisons with known reference noise sources must be made in order to keep the amplification and the bandwidth stable and to eliminate the influence of drifts and detector and circuit noise. A corresponding project is currently pursued by NIST and the Measurement Standards Laboratory in New Zealand. The main problem is the long measuring time that is required for low uncertainties. To achieve an uncertainty in the range of $1\cdot10^{-5}$ for a bandwidth of 20 kHz, a measuring time of about five weeks is necessary. Here, the determination of the Boltzmann constant clearly reaches its bounds.

2.4. Doppler broadening thermometer

A further method to determine k by means of laser spectroscopy has been proposed only recently. It is based on the measurement of the Doppler broadening of an absorption line by means of the movement of gas particles in a cell at a homogeneous temperature, see figure 3. Information on the temperature (Table 1) is gained from the width of the absorption profile which is scanned by means of tuneable laser radiation.

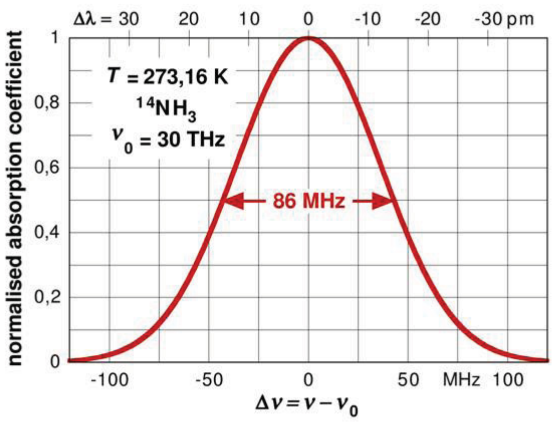

Figure 3: Doppler-broadened absorption line profile for ammonia $^{14}NH_3$ at T_{TPW} assuming a central frequency of $\nu_0 = 30$ THz.

At the Université Paris Nord, experiments have been carried out with a CO_2 laser at an ammonia line at 30 THz. A relative standard uncertainty for k of approximately $3.8\cdot10^{-5}$ could be estimated [8]. In a second project, the Second University of Naples and the Polytechnic of Milan use high-resolution spectroscopy at a CO_2 line with a diode laser in the near infrared range. At present, the relative uncertainty is $1.6\cdot10^{-4}$ [9]. A third experiment is being developed at the Institute Dansk Fundamental Metrology. Due to enormous difficulties with the separation of the Doppler broadening from other line shape modifications, which are caused by interaction of the particles, a reduction of the uncertainty to below $1\cdot10^{-5}$ is unlikely.

3. CONSEQUENCES OF THE NEW DEFINITION

The formulation of the new definition of the kelvin could be as follows [2]: The kelvin is the change of the thermodynamic temperature T which corresponds to a change of the thermal energy kT of exactly $1.38065XX\cdot10^{23}$ joule. This formulation is in analogy to the definition of the meter selected in 1983 and can be considered as an explicit definition of the unit itself. As an alternative, a formulation which is explicitly related to a fundamental constant is conceivable: The kelvin, the unit of the thermodynamic temperature T, is defined in such a way that the Boltzmann constant has exactly the value of $1.38065XX\cdot10^{23}$ J/K. Both formulations are practically equivalent.

What are the consequences of such a new definition? First of all the practical effects will not be spectacular, they should not even be felt, so that international metrology as has been applied so far can continue to function undisturbed and the development of the worldwide division of labour and production continues unaffected. Anything else would create enormous costs. To achieve this, the CIPM Consultative Committee for Thermometry is already working on a "mise en pratique" - a recommendation for implementation - containing not only recommendations for the direct measurement of the thermodynamic temperature T as well as the defining texts of the still valid International Temperature Scales ITS-90 and PLTS-2000 [10, 11], but also a discussion of the differences $T - T_{90}$ and $T - T_{2000}$ with their uncertainties. T_{90} and T_{2000} are temperature values which are determined according to the individual scale specifications. This procedure permits direct thermodynamic temperature measurements far from the triple point of water, e.g. at high temperatures where the radiation thermometer can be used both as an interpolation instrument of the ITS-90 and as a primary thermometer. In future, this will help to substantially reduce the uncertainties which, e.g. at the highest fixed point of the ITS-90 at 1358 K, are almost one thousand times larger than the reproducibility of the triple point of water.

In the temperature range around the triple point of water, T_{TPW}, which is important in practice, the ITS-90 will still keep its right to exist. However, the triple point of water, which is currently - by definition - provided with an exact temperature, will lose its outstanding position. It will then be a temperature fixed point like any other, which has exactly the same uncertainty as the Boltzmann constant at the time of its definition. A relative uncertainty of $1\cdot10^{-6}$ corresponds to 0.27 mK.

4. SUMMARY AND OUTLOOK

Figure 4 shows a summary of the published determinations of the Boltzmann constant since 1988. The determination by acoustic gas thermometry (AGT) by NIST [12] provides the basis of the 2006 accepted value. Motivated by the recommendation of the CIPM in 2005, numerous new experiments have subsequently been set up. In 2007, refractive index-gas thermometry (RIGT) at NIST [13] provided a numerical value with a relative standard uncertainty of $9.1 \cdot 10^{-6}$. From measurements with a non-adapted low-temperature version of the dielectric constant gas thermometer (DCGT) of PTB, a preliminary value of the Boltzmann constant can be derived with a relative uncertainty of $3.0 \cdot 10^{-5}$. As has been mentioned before, initial Doppler broadening measurements (DBT, UniNa) of the Italian group achieved uncertainties of $1.6 \cdot 10^{-4}$ [9]. The Doppler absorption curves (DBT, LPL) at the Université Paris Nord were successively analysed with two different line profiles and published in 2009 and 2010 [8]. The relative difference in the value of the Boltzmann constant of $3.7 \cdot 10^{-5}$ illustrates the considerable problems of understanding the line shape for the same input data. A complete uncertainty budget has not been published, it can, however, be estimated at approximately $3.8 \cdot 10^{-5}$.

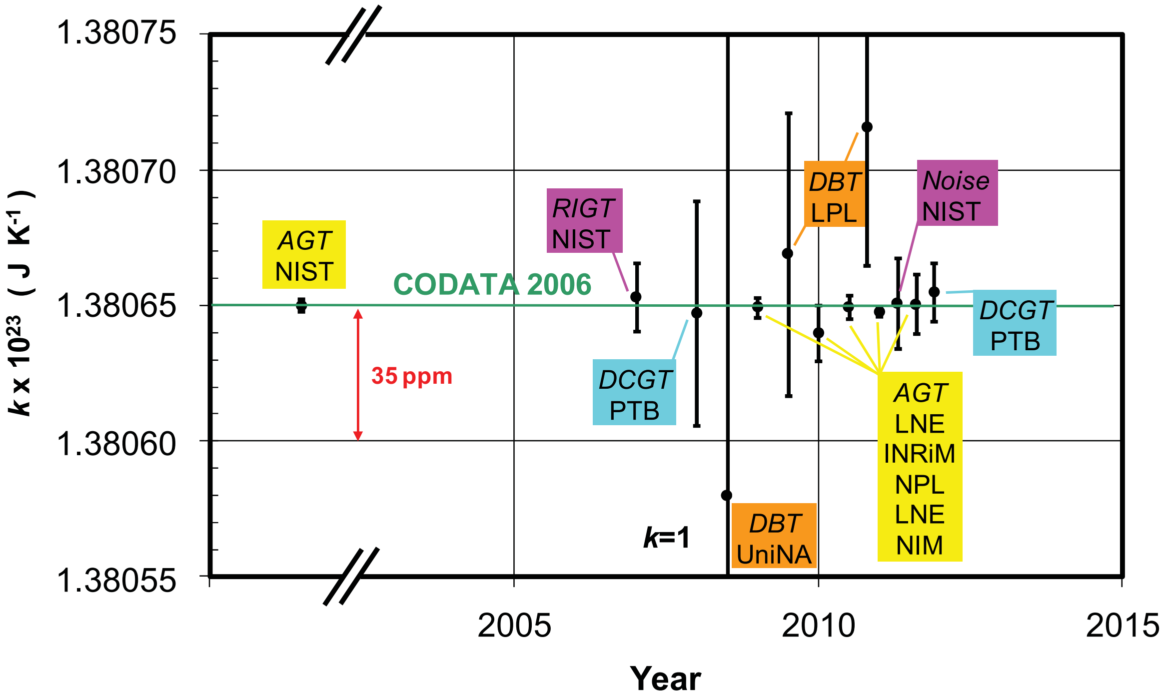

Figure 4: Overview of the determinations of the Boltzmann constant k or the universal gas constant $R = k \cdot N_A$ since 1988. Explanations of the abbreviations can be found in section 4. The bars describe the standard uncertainties. The green line indicates the numerical value of k which has been 2006 internationally recommended by CODATA.

The most accurate newer values of the Boltzmann constant, which were published in 2009 and 2010, were achieved by the similarly set up acoustic gas thermometers (AGT) at the French national institute LNE [14, 15], at the Italian INRiM [16] and at the British NPL [17]. The relative standard uncertainties amount to $2.7 \cdot 10^{-6}$ and to remarkably low $1.2 \cdot 10^{-6}$, respectively, $7.5 \cdot 10^{-6}$ and $3.1 \cdot 10^{-6}$ respectively. First determinations have been achieved by the Johnson noise thermometry experiment at NIST [18], the acoustic gas thermometry experiment at the Chinese state institute NIM [19], which has been launched only recently, and by the new dielectric constant gas thermometry experiment at PTB [7]. The relative uncertainties are $12.1 \cdot 10^{-6}$, $7.9 \cdot 10^{-6}$ and $7.9 \cdot 10^{-6}$, respectively.

The graph shows that so far, no *independent* method has been able to confirm the AGT measurements of NIST at the required level of uncertainty. Therefore, the international Consultative Committee for Thermometry (CCT) recommended CIPM in 2010 to wait for at least two further results - which will have been achieved by means of independent methods - before re-defining the kelvin. The CIPM followed this recommendation, also due to the discrepancies which occurred with the determination of Planck's constant for the re-definition of the kilogram, and has accordingly approved the new definitions for the kilogram, ampere, mole and kelvin only in principle. However, it cannot be implemented until enough consistent measurements are available.

For 2013, the CCT is now expecting an averaged value for k with a relative standard uncertainty well below 10^{-6} which is based on various experiments with at least two different methods (acoustic gas thermometer and dielectric constant gas thermometer). Besides, the noise thermometer and perhaps also the Doppler broadening thermometer should be able to provide an additional confirmation, though with larger uncertainties. Thus, there is enough time to make use of the promising potentials of the different measurement methods.

Due to the significant progress achieved with the development of the described primary thermometers, the Boltzmann constant can be determined with such precision that the new definition of the kelvin will be possible by means of a single fixing of its numerical value. The essential consequences of the new definition of the kelvin are of a long-term nature because a fundamental constant - instead of a material property - is now taken as scale. The system of units would thus be indefinitely stable. This objective is worth the effort made world-wide.

5. REFERENCES

[1] Recommendation 1 (CI-2005) of the CIPM (english version: www.bipm.org/cc/CIPM/Allowed/94/CIPM-Recom1CI-2005-EN.pdf)

[2] I.M. Mills, P.J. Mohr, T.J. Quinn, B.N. Taylor, E.R. Williams, "Redefinition of the kilogram, ampere, kelvin and mole: a proposed approach to implementing CIPM recommendation 1 (CI-2005)", Metrologia **43** pp. 227-246 (2006)

[3] P.J. Mohr, B.N. Taylor, D.B. Newell, "CODATA recommended values of the fundamental physical constants: 2006", Rev. Mod. Phys. **80** pp. 633-730 (2008)

[4] B. Fellmuth, J. Fischer (editors), Talks of the 221. PTB Seminar "Workshop on Progress in Determining the Boltzmann Constant", Bericht PTB-Th-3, Braunschweig, ISBN 978-3-86509-684-5 (2007)

[5] B. Fellmuth, Ch. Gaiser, J. Fischer "Determination of the Boltzmann Constant – status and prospects", Meas. Sci. Technol. **17** pp. R145-R159 (2006)

[6] C. Gaiser, B. Fellmuth, N. Haft, "Dielectric-constant gas-thermometry scale from 2.5 K to 36 K with ^{3}He , ^{4}He and neon", Int. J. Thermophys. **31** pp. 1428–1437 (2010)

[7] B. Fellmuth, J. Fischer, C. Gaiser, O. Jusko, T. Priruenrom, W. Sabuga, T. Zandt, "Determination of the Boltzmann constant by dielectric-constant gas thermometry", Metrologia (2011) accepted

[8] C. Lemarchand, K. Djerroud, B. Darquié, O. Lopez, A. Amy-Klein, C. Chardonnet, Ch.J. Bordé, S. Briaudeau, C. Daussy, "Determination of the Boltzmann Constant by Laser Spectroscopy as a Basis for Future Measurements of the Thermodynamic Temperature", Int. J. Thermophys. **31** pp. 1347-1359 (2010)

[9] G. Casa, A. Castrillo, G. Galzerano, R. Wehr, A. Merlone, D. Di Serafino, P. Laporta and L. Gianfrani, "Primary Gas Thermometry by Means of Laser-Absorption Spectroscopy: Determination of the Boltzmann Constant", Phys. Rev. Lett. **100** 200801 (2008)

[10] Mise en pratique for the definition of the kelvin, http://www.bipm.org/utils/en/pdf/MeP_K.pdf

[11] D.C. Ripple, R. Davis, B. Fellmuth, J. Fischer, G. Machin, T. Quinn, P. Steur, O. Tamura, D.R. White, "The Roles of the Mise en Pratique for the Definition of the Kelvin", Int. J. Thermophys. **31** pp. 1795–1808 (2010)

[12] M.R. Moldover, J.P.M. Trusler, T.J. Edwards, T.J. Mehl and R.S. Davis, "Measurement of the universal gas constant R using a spherical acoustic resonator", J. Res. Natl. Bur. Stand. **93** pp. 85-114 (1988)

[13] J.W. Schmidt, R.M. Gavioso, E.F. May, and M.R. Moldover, "Polarizability of Helium and Gas Metrology", Phys. Rev. Lett. **98** 254504 (2007)

[14] L. Pitre, C. Guianvarc'h, F. Sparasci, A. Guillou, D. Truong, Y. Hermier, M. Himbert, "An improved acoustic method for the determination of the Boltzmann constant at LNE-INM/CNAM", C. R. Physique **10** pp. 835-848 (2009)

[15] L. Pitre, F. Sparasci, D. Truong, A. Guillou, L. Risegari, M. E. Himbert, "Measurement of the Boltzmann Constant k_B using a Quasi-Spherical Acoustic Resonator", Int. J. Thermophys. (2011) in press

[16] R.M. Gavioso, G. Benedetto, P.A. Giuliano Albo, D. Madonna Ripa, A. Merlone, C. Guianvarc`h, F. Moro, and R. Cuccaro, "A determination of the Boltzmann constant from speed of sound measurements in helium at a single thermodynamic state", Metrologia **47** pp. 387-409 (2010)

[17] G. Sutton, R. Underwood, L. Pitre, M. de Podesta, S. Valkiers, "Acoustic Resonator Experiments at the Triple Point of Water: First Results for the Boltzmann Constant and Remaining Challenges", Int. J. Thermophys. **31** pp. 1310-1346 (2010)

[18] S.P. Benz, A. Pollarolo, J. Qu, H. Rogalla, C. Urano, W.L. Tew, P.D. Dresselhaus, D.R. White, "An electronic measurement of the Boltzmann constant", Metrologia **48** pp. 142-153 (2011)

[19] J.T. Zhang, H. Lin, X.J. Feng, J. P. Sun, K.A. Gillis, M.R. Moldover, Y.Y. Duan, "Progress toward redetermining the Boltzmann constant with a fixed-path-length cylindrical resonator", Int. J. Thermophys. DOI 10.1007/s10765-011-1001-3 (2011)