On new definitions of SI base units. Why is the “atomic” kilogram preferable

K.A. Bronnikov\textsuperscript{a,b,c,1}, V.D. Ivashchuk\textsuperscript{a,b,2}, M.I. Kalinin\textsuperscript{a,3}, V.V. Khruschov\textsuperscript{a,d,4}, S.A. Kononogov\textsuperscript{a,5}, and V.N. Melnikov\textsuperscript{a,b,6}

\textsuperscript{a} Center for Gravitation and Fundam. Metrology, VNIIMS, Ozyornaya ul. 46, Moscow 119361, Russia;
\textsuperscript{b} Institute of Gravitation and Cosmology, PFUR, ul. Miklukho-Maklaya 6, Moscow 117198, Russia;
\textsuperscript{c} I. Kant Baltic Federal University, ul. Al. Nevskogo 14, Kaliningrad 236041, Russia;
\textsuperscript{d} National Research Center Kurchatov Institute, pl. Akademika Kurchatova 1, Moscow 123182, Russia

Abstract

We discuss the role of fundamental constants and measurement data for the Planck, Avogadro and Boltzmann constants and the elementary electric charge in connection with the planned transition to new definitions of four base SI units (the kilogram, mole, ampere and kelvin) in terms of fixed values of these constants. It is proposed to choose a new definition of any base SI unit in terms of a particular fundamental physical constant using a number of criteria, or principles, such as succession relative to the current SI, a sufficient stability of the new unit standards, and concordance between physical dimensions of the unit and the corresponding fundamental constant. It is argued that a redefinition of the kilogram and mole by fixing the values of the atomic mass unit and the Avogadro constant satisfies all these criteria and bears some more advantages against the version with fixed Planck constant: a well founded approach to definition of the ampere and the opportunity to preserve the current relationship between definitions of the mole and the kilogram. It is also argued that the kelvin can be redefined independently of the other three units.

Keywords: redefinition of SI base units, fundamental physical constant, dimension of a physical quantity, instability of the International Prototype of the Kilogram.

1 Introduction

There are at present three main unresolved problems in modern physics:
— unification of the four known physical interactions including gravity;
— the present acceleration of the universe, the dark energy (DE) and dark matter (DM) problems;
— possible variations of fundamental physical constants (FPC): the fine structure and gravitational constants, electron to proton mass ratio etc.

The constants we meet in physical theories characterize the stability properties of different types of matter, objects, processes, classes of processes and so on. These constants are important because they are the same under diverse circumstances, at least within the measurement uncertainties we have achieved nowadays. That is why they are called FPCs and that is why they,
or their combinations, can be used as natural scales determining the basic units. With scientific progress some theories are replaced by more general ones with their own constants, and new relations emerge between different constants. Thus what we can discuss is not the absolute choice of FPCs but only a choice corresponding to the present situation in the physical sciences [1].

At present, the theory of electroweak interactions has a reliable confirmation in accelerator experiments with elementary particles. There exist a sufficiently well developed and confirmed theory of its unification with the strong interaction, the so-called Standard Model, and the well-tested (mainly in the Solar System) theory of gravity, Einstein’s General Relativity (GR). In cosmology, with a rapidly developing observational base and its theoretical interpretation, an important role belongs to the Standard Cosmological Model (the spatially flat Friedmann model with the cosmological constant ($\Lambda$CDM) and its multiple modifications and extensions. All these theories, each with its own constants, have certain problems [2], and a further development of physics, especially while solving the above major problems, will probably change the presently chosen set of FPCs. When it can happen, we do not know.

The existing systems of units of physical quantities are a part of the necessary toolkit of science, and, as any tools, they should adequately correspond to the present-day state of the art. Redefinition of the set of base units of the International System of Units (SI), being now under preparation [3], can be considered as a response to this challenge. The planned revision of SI rests on the proposal to define the base SI units by fixing the exact values of the corresponding FPCs, following the principle that was already used in the definition of the metre in 1983.

This revision is under discussion since 2005, and it has been proposed, in particular, to fix with zero uncertainty the values of the constants $h$, $e$, $k$, and $N_A$ and on this basis to redefine the kilogram, ampere, kelvin and mole [3–10]. One of the reasons for changing the existing definitions of these units is the revealed temporal instability of the International Prototype of the Kilogram (IPK), being on the level of $5 \times 10^{-10}$ kg per year [11].

Employment of exact FPC values has a great significance in metrology [12–16], and the proposals to redefine a number of SI units on the basis of fixed FPC values have been supported by metrological agencies, workshops and conferences [3, 5, 7–9].

Why was it impossible to introduce such new definitions as soon as their necessity was realized? The main obstacle was the insufficient accuracy of the current knowledge of the relevant FPCs.

The current situation with a transition to new definitions of the kilogram and the mole, the most important one is achieving the level of $2 \times 10^{-8}$ for the relative standard uncertainty $u_r$ for the values of the Planck and Avogadro constants and a consistency between their values obtained
by different methods with $u_r \simeq 5 \times 10^{-8}$. However, there are different versions of such new definitions, and even after meeting the above requirements, the question of choosing a specific version of definitions of the kilogram and mole will remain open. For example, for the unit of mass there are versions based on fixing the Planck constant and those based on fixing the atomic mass unit. In the present paper, it is suggested to choose a new definition of a particular unit of measurement with the aid of a number of criteria and principles. When choosing a new definition of the mass unit, one should take into account Decision G1 of the Consultative Committee on Mass and Related Quantities (CCM) adopted at a session in 2010 [17], where it was suggested to soften the previously adopted recommendations of BIPM and the 23ed CGPM for replacing the IPK [5, 8] as follows:

— at least three independent experiments, including work both from watt balance and from International Avogadro Coordination projects, yield values of the relevant constants with relative standard uncertainties not larger than 5 parts in $10^{8}$. At least one of these results should have a relative standard uncertainty not larger than 2 parts in $10^{8}$;

— for each of the relevant constants, values provided by the different experiments be consistent at the 95% level of confidence,

— traceability of BIPM prototypes to the international prototype of the kilogram be confirmed.

These constraints are the weakest possible since a further increase in $u_r$ of measuring the Planck and Avogadro constants would lead to a violation of the existing practice of high-precision mass measurements for class E1 masses [18].

A condition for passing over to a new definition of the kelvin is to achieve a level within $u_r(k) \leq 1 \times 10^{-6}$ in measurements of the Boltzmann constant $k$. Before 2010, the $k$ value, adopted as the most accurate one, was obtained in the NIST experiment of 1988, with an uncertainty $u_r(k) = 1.7 \times 10^{-6}$ [19,20]. After 2010, the effort of a number of research groups from USA, England, Germany, Italy and France led to important results in improving the accuracy of experimental facilities for measuring the Boltzmann constant.

A transition to a new definition of the ampere using a fixed value of the elementary charge depends, on the one hand, on which decision will be made about the new definition of the kilogram (more precisely, whether or not the Planck constant value will be fixed); on the other hand, it is expected that a quantum standard of the ampere will be created on the basis of direct counts of electrons passing a certain surface, [21–31], which will allow for introduction of an independent definition of the ampere.

The paper is organized as follows. Section 2 outlines the recent results of measurements of the Planck, Avogadro and Boltzmann constants and the elementary electric charge. Section 3 suggests and discusses the criteria for a preferable choice of new definitions of the base SI units. Section 4 discusses the existing problems with a transition to a new definition of the kilogram using a fixed value of $h$, known as the “electric kilogram”. In Section 5, on the basis of the criteria formulated in Section 3, we suggest to perform a redefinition of the SI units with such a set of FPCs that a new definition of the kilogram and the mole will employ fixed values of the atomic mass unit (instead of a fixed value of the Planck constant) and the Avogadro constant (the version known as the “atomic kilogram”). Section 6 discusses a physical foundation of fixing the value of the Boltzmann constant and a possible transition to a new definition of the kelvin in the nearest years. Section 7, the conclusion, summarizes our main proposals. Expansions of abbreviated names of institutions mentioned in the text are given before the bibliography.
2 Measurement data

At present, three experiments for measuring the Planck and Avogadro constants satisfy the first condition of CCM Recommendation G1 of 2010 [17]. The results of new measurements of the Planck constant at NIST with a watt balance (w.b.) were recently published [32],

\[ h_{\text{NIST}-14-w.b.} = 6.62606979(30) \times 10^{-34} \text{ J s}, \]

with \( u_r = 4.5 \times 10^{-8} \), and those of the NRC project [33],

\[ h_{\text{NRC}-14-w.b.} = 6.62607034(12) \times 10^{-34} \text{ J s}, \]

with \( u_r = 2 \times 10^{-8} \). These new results in watt-balance experiments, as well as the result obtained in the International Avogadro project (IAC) in 2011 [34],

\[ h_{\text{IAC}-11-28Si} = 6.62607014(20) \times 10^{-34} \text{ J s}, \]

also satisfy the second condition of Recommendation G1 of CCM because the difference \( h_{\text{IAC}-11-28Si} - h_{\text{NIST}-14-w.b.} \) has turned out to be \( 5.3 \times 10^{-8} h \), while \( h_{\text{NRC}-14-w.b.} - h_{\text{IAC}-11-28Si} \) is of the order of \( 2 \times 10^{-8} h \), and \( h_{\text{NRC}-14-w.b.} - h_{\text{NIST}-14-w.b.} \) is of the order of \( 7.3 \times 10^{-8} h \). Condition 2 (G1 CCM) is fulfilled because each of the differences \( h(i) - h(j) \) is smaller by absolute magnitude than twice the combined standard uncertainty, \( 2[(u_r(h(i))h(i))^2 + (u_r(h(j))h(j))^2]^{1/2} \), \( i, j = 1, 2, 3(i < j) \).

The results of the Avogadro project [34] were confirmed with high accuracy by new silicon molar mass measurements at NMIJ [35] and NIST [36], for a review see also [37].

Let us note that CODATA gives for the Planck constant [38] the value

\[ h_{\text{CODATA-2010}} = 6.62606957(29) \times 10^{-34} \text{ J s}, \]

with \( u_r = 4.4 \times 10^{-8} \), where the old result of NIST (2007) has been used.

When obtaining the Planck constant value in the Avogadro project, the value of \( N_A \), measured in the same experiment, was used [34]:

\[ N_{A(\text{Avogadro-2010})} = 6.02214084(18) \times 10^{23} \text{ mole}^{-1}, \]

with \( u_r = 3 \times 10^{-8} \), and the new value of the Planck molar constant [38]

\[ N_A h_{\text{CODATA-2010}} = 3.9903127176(28) \times 10^{-10} \text{ J s mole}^{-1}, \]

with \( u_r = 0.7 \times 10^{-9} \), obtained from the well-known relation

\[ N_A h = A_r(e) M_u c^2/(2R_\infty), \tag{2.1} \]

where the molar mass constant \( M_u = N_A m_u \) coincides in the ("old") SI with \( M_{u0} = 1 \text{ g/mole} \) (\( m_u = m^{(12)\text{C}}/12 \) is the atomic mass constant), \( A_r(e) \) is the relative atomic mass of the electron, \( R_\infty \) is the Rydberg constant, \( c \) is the speed of light in vacuum, and \( \alpha \) is the fine structure constant.

The calculation of the Planck molar constant in CODATA-2010 has used the value of \( \alpha \) such that

\[ \alpha^{-1}_{\text{CODATA-2010}} = 137.035999074(44), \]

with \( u_r(\alpha) = 3.2 \times 10^{-10} \) and the electron atomic mass value

\[ A_r(e) = 5.4857990946(22) \times 10^{-4}, \text{ with } u_r(A_r(e)) = 4 \times 10^{-10}. \]
A contribution of the uncertainty of the Rydberg constant, \( u_r(R_\infty) = 5 \times 10^{-12} \) into the relative standard uncertainty \( u_r(N_A h) \) is negligibly small.

It should be noted that the quantity \( u_r(N_A h) \) also determines a constraint on the correction factor \( \kappa \), emerging in the new version of the definitions of the kilogram and mole based on fixed values of \( h \) and \( N_A \):

\[
\kappa = M_u/M_{u0} - 1 = N_A m(^{12}\text{C})/(12 M_{u0}) - 1,
\]

which is estimated as \( |\kappa| < 1.4 \times 10^{-9} \) with 95% confidence [38].

The emergence of the new parameter \( \kappa \) in the new SI is strongly criticized in the literature, see [42–45] and references therein. The main arguments come from the chemical and educational communities. The introduction of such a new and unnecessary entity is evidently out of accord with the famous Occam’s razor principle.

At measurements of the Avogadro constant with the aid of silicon crystal balls, the following relation is used [34]:

\[
N_A = 8M/(\rho a^3),
\]

where \( \rho \), \( M \) and \( a \) are the density, molar mass and lattice constant of silicon, respectively. In this method, the main contributions to the full uncertainty budget are connected with measurements of the accuracy of the ball’s spherical surface and its roughness (65.8%), the mass of the ball’s surface layers (16.7%), the crystal lattice parameter (8.7%) and the molar mass of silicon (4.9%). Altogether, these contributions, among which the largest one is related to the inaccuracy of determining the ball’s diameter, did not allow for achieving the total \( u_r \) of \( 2 \times 10^{-8} \), and as a result of completing the second stage of Avogadro international project at the end of 2010, the value of the Avogadro constant was determined with \( u_r \) equal to \( 3 \times 10^{-8} \) [34].

A large role in rising the accuracy of the final result belongs to corrections that emerge due to deflections of the basic parameters of silicon crystal balls from their assumed perfect behaviour. Such deflections include impurities, crystal lattice defects and inhomogeneities of the surface layer that affect the measured values of almost all parameters. Thus, for instance, the uncertainties emerging while measuring the mass of a surface layer of the ball lead to the second largest contribution to the full uncertainty after the error in measuring the ball diameter; this contribution is close to 17% [34]. The impurities mostly consist of carbon, oxygen and boron. In addition, there appeared impurities which had not been anticipated at the beginning of the experiment, they emerged at ball surface polishing and consisted of metallic contamination of copper and nickel. The metallic contaminations very strongly affected the optical characteristics of the surface layer and prevented the precision interferometric measurements.

However, the results obtained in the Avogadro project was verified at PTB, where the value of the Avogadro constant was found after removal of copper and nickel from the surface of the silicon ball IAC \(^{28}\text{Si AVO28-S8} \). After wet etching and repeated polishing of the ball’s surface, its diameter decreased by 300 nm and its mass by approximately 9 mg. The \( N_A \) value measured at PTB coincided with that previously obtained in the Avogadro project within \( u_r = 3 \times 10^{-8} \). Moreover, a measurement of the contributions of extraneous chemical elements in the silicon specimen used for fabrication of the ball AVO28-S8, conducted at INRIM [46], also confirms the confidence of \( u_r = 3 \times 10^{-8} \) in the result of the Avogadro project.

The measurements performed at NIST in May 2010 have created a shift in the \( h \) value:

\[
(h/h_{90} - 1) = 97(37) \times 10^{-9} \] [32]. A final correction of the NIST-14 result has followed from recalibration of the platinum-iridium standard K85 at BIPM, which has led to a mass increase of K85 by \( 40 \times 10^{-9} \), and this in turn led to \( h/h_{90} - 1 = 137 \times 10^{-9} \), which is close to the result of [32], but the authors were unable to find a satisfactory explanation of this shift.
Let us recall that in the case of a radially directed magnetic field $B$, for the current value $I$ in a conducting coil with a conductor of length $L$, at the “force” phase of the experiment, it holds $ILB = mg$, while the “velocity” phase of the experiment is described by the relation $U = BLv$, where $v$ is the velocity in the vertical direction, and $U$ is the inductive electromotive force. As a consequence, we obtain the well-known relation $IU = mgv$, which for $I = U' / R$ can be rewritten in the form

$$mv = UI = \frac{U_{90}U'_{90}K_{J-90}^{2}R_{K-90}}{R_{90}} h,$$

where $K_{J-90}$ and $R_{J-90}$ are certain conditionally adopted constants which in general do not coincide with the Josephson and von Klitzing constants, $K_{J} = 2e / h$ and $R_{K} = h / e^2$. It is assumed here that $U$ and $U'$ are measured using the voltage standards on the basis of the Josephson effect and giving the values $U_{90}$ and $U'_{90}$, respectively, while the resistance $R$ is measured by an ohmmeter based on the quantum Hall effect, giving as a result $R_{90}$.

Thus the new result of measuring $h$ published by NIST [32] in 2014 points at the existence of significant systematic errors in the previous NIST result (2007); it also confirms the result of the Avogadro project (2011).

Unlike the NIST-3 experiment described above, the watt balance experiment of the Canadian group (NRC) used a permanent magnet. Main contributions to the $u_r$ value are here connected with the errors of “mass exchange”, $1.7 \times 10^{-8}$, the knife blade hysteresis, $1 \times 10^{-8}$, the buoyancy force, $0.1 \times 10^{-8}$, magnetization, $0.1 \times 10^{-8}$, and “susceptibility”, $0.1 \times 10^{-8}$ [33].

It should be noted that the reliability of the NIST-2014 result of measuring the Planck constant was verified to a large extent in the process of collaboration between NIST and NRC. The result of Canadian researchers in $h$ measurement with a watt balance, $h$(NRC-14-w.b.), published in 2014, is of great importance since it gives $u_r(h)$ equal to $2 \times 10^{-8}$ and differs from the result of the Avogadro project by the same amount, whereas the difference between $h$(NRC-14-w.b.) and $h$(NIST-14-w.b.), equal to $(7.3 \times 10^{-8} \ h)$, is smaller that twice the combined standard uncertainty equal to $(9.85 \times 10^{-8} \ h)$. Therefore, the second condition of CCM G1 is fulfilled, which makes it possible to begin the redefinition of SI units in the nearest years (according to [9], in 2018).

The BIPM recommendations and Resolutions of the 23rd CGPM of 2007 on the transition to new definitions of a number of base SI units have promoted an increased activity of theoretical and experimental studies in thermometry and the related branches of physics and to an improvement of methods and means of primary thermometry for measuring the Boltzmann constant with accuracies exceeding $10^6$. The experimental groups at NPL (England), PTB (Germany), LNE-CNAM (France), NIST (USA), INRIM (Italy) have achieved a substantial progress in improving the accuracy of measuring the Boltzmann constant [47–54]. The contributions of various experimental factors to the uncertainty budget of measuring $k$ were thoroughly studied and estimated quantitatively, especially for acoustic gas thermometers. This has led to a substantial decrease in the measurement uncertainties when using different types of primary thermometers. For acoustic thermometers, $u_r$ was lowered up to $1 \times 10^{-6}$ and less, for other types of thermometers (on the basis of measuring the dielectric constant of a gas, the Doppler broadening of gas absorption spectra, noise thermometry) up to $\sim 10^{-5} \div 10^{-4}$.

The authors of [18] (2011) obtained a value of $k$ with the uncertainty $u_r(k) = 1.24 \times 10^{-6}$. At NPL, using an acoustic gas thermometer with a quasispherical cavity, a result was obtained in 2013 with $u_r(k) = 0.71 \times 10^{-6}$ [34]. At present, according to CODATA-2010 [38], a value of the Boltzmann constant is adopted as $k = 1.3806488(13) \times 10^{-23}$ J/K, with the uncertainty $u_r(k) = 0.91 \times 10^{-6}$, and so the CGPM demands are already fulfilled.
The introduction of a new definition of the ampere with the aid of a fixed value of the elementary charge is also one of the basic tasks of the planned reform of the SI system. As is well known, up to now, the currently official definition of the ampere in SI is obsolete, resting on the value of a force acting between parallel infinite conductors with a current, whereas the practice of precision electric measurements employs the macroscopic quantum effects, the quantum Hall effect and the Josephson effect, characterized by the von Klitzing ($R_K$) and Josephson ($K_J$) constants, respectively:

$$R_K = \frac{h}{e^2}, \quad K_J = \frac{2e}{h}.$$  \hfill (2.3)

The most frequently discussed version of the reform contains a proposal to fix the values of $h$ and $e$ with zero uncertainty, hence, according to (2.3) also the values of the constants $K_J$ and $R_K$. As a result, the units of charge, the coulomb, and the unit of current, the ampere equal to a coulomb per second, will also be fixed, thus bringing the electric part of the SI system to correspondence with the modern practice of measurements.

However, this scenario faces a number of problems. First, there is some reasonable doubt concerning the validity of equations (2.3) for systems with a small number of electrons, and for such systems it is necessary to have an independent experimental confirmation of these relations.

Second, such a confirmation is expected in the nearest years on the basis of single-electron tunneling [21]; however, this phenomenon will by itself lead to an independent version of the definitions of the electric charge and current (in other words, to emergence of a quantum standard of the ampere), which creates a problem of choosing the formulations of the corresponding definitions in the SI system. Indeed, a direct count of the number of electrons crossing a certain section of the conductor per unit time directly connects the system unit of charge (the coulomb) with the elementary charge. The problem of agreement between different versions of definitions for the coulomb and the ampere has acquired the conditional name of the "quantum metrological triangle", whose "closure" is one of the purposes of the single-electron tunneling experiments. To put it simpler, to "close" the triangle means to confirm the validity of Ohm’s law for three quantities: the Josephson voltage, the Hall resistance, and the single-electron tunneling current.

Lastly, third, a new definition of the ampere should become a constituent of the unified system of definitions in the new SI that rests on fixed values of a certain set of FPCs. However, in connection with the problem of choosing a new definition for the kilogram (see Sections 4 and 5 of the present paper), in this set of constants, the Planck constant $h$ may be lacking. This circumstance even more increases the value of a definition of the ampere which will not depend on the $h$ value and will be based on precise counts of elementary charges crossing a section of a conductor with current per unit time.

While planning the SI revision, concerning the ampere, the task was formulated to obtain $u_t$ of current measurements within $10^{-8}$. Studies and experiments aimed at achieving this goal are being conducted in many laboratories of the world. Let us mention, in particular, such perspective trends as hybrid (metal-semiconductor) electron pumps [25], electron pumps with graphene quantum dots [26], and the European program “Quantum ampere — realization of the SI ampere”, whose intermediate results have been published in [27–30]. The available information indicates that, despite significant success of the researchers, a new definition of the ampere on the basis of a fixed value of the elementary charge cannot be introduced too soon. Thus, one can notice that by now measurements of the currents are not considered with uncertainties $u_t(J)$ smaller than $10^{-7}$. An accuracy increase of one more order of magnitude will naturally require new effort and time.
3  Criteria for an optimal choice of constants with fixed values for redefinitions of measurement units

How to choose the set of FPCs and their fixed values in an optimal way for creating new definitions of SI units? At first sight it seems that a physical constant, whose value is determined by suitable measurements for redefinition of a certain SI unit, cannot be fixed because its value inevitably contains a measurement uncertainty. However, if the uncertainty is smaller than a prescribed limit, which depends on a maximum accuracy of measurements conducted with the unit under consideration, then for a new definition of this unit it is quite admissible to fix the value of the corresponding constant, unless this procedure can lead to a contradiction with the usage of other constants with fixed values. It is also clear that the status of any FPC is not absolute and can change due to generalization of a relevant theory or when the measurement accuracy increases.

Anyway, the key requirement to the new SI is that it should not aggravate the situation in any respect for any users as compared with the old SI. This means, above all, a necessary succession with respect to the old SI, which implies establishing the same set of base and derivative units and the same values of all units as they exist by the day of revision in order that the whole enormous set of the existing measurement data could be preserved without recalculation.

Second, evidently, the revision of SI should not worsen the stability properties of the standards of any units against the old ones. In this respect, it is necessary to recall the detected temporal instability of the IPK copies for 100 years \(11\) on the level of \(5 \times 10^{-10}\) per year. So the new BIPM prototypes should have a confirmed temporal instability not worse than that, and this requirement should hold for any new prototype of the kilogram at any time and place. It is clear that similar requirements concern all base SI units.

We here do not discuss FPC variations on the cosmological scale of times and distances closely related to the above-mentioned problems of unification of interactions, dark energy and dark matter (see, e.g., \(39–41\) and references therein). Such variations, if any, are too small in the present epoch and cannot change the stability of the basic standards. But they are of great importance for further development of fundamental interaction theories \(1, 40\).

Third, for establishing a relationship between the system of measurement units and physical theories, it is desirable that the number of fixed constants were minimum possible, and that the relation between the FPC used and the corresponding unit were as simple as possible. The same conditions are desirable for successful teaching of the fundamentals of metrology at universities and colleges. This goal is achieved if the base measurement unit and the corresponding FPC have the same physical dimension. That is, if \([D]_{BU}\) is the dimension of the base unit and \([D]_{FPC}\) is that of the FPC to be fixed, it is desirable that

\[
[D]_{BU} = [D]_{FPC}. \tag{3.1}
\]

However, a literal application of this principle makes it impossible to have such base units as the meter and the ampere. Instead, the velocity and electric charge units will be base units, contrary to the first requirement above and also to the international standard ISO/IEC 80000 \(55\) which determines the set of base physical quantities in the International System of Quantities (ISQ). To preserve the same set of base units of the new SI, the condition (3.1) for choosing the FPC should be relaxed \(56\). The extended criterion can be formulated as follows: a base measurement unit is defined with the aid of an FPC with the same dimension or the one that differs from it by a certain power of time:

\[
[D]_{BU} = [D]_{FPC} \times [T]^d, \tag{3.2}
\]
where \( d \) is a rational number. Then the unit of length can be, as before, defined by fixing the velocity of light, and a new definition of the ampere can rest on a fixed value of the elementary charge. Taking into account the all-time high accuracy in measuring times or frequencies, the possible presence of the additional factor \([T]^d\), which is necessary for preserving succession with the old SI, will not affect the reproduction accuracy of the corresponding unit.

The maximum possible simplicity of the new SI also assumes that, if possible, the base measurement units should be mutually independent, and that no new quantities (like the correction factor \( \kappa \) in Eq. (2.2) above) should be introduced at the transition to new definitions. It can be said in advance that, as follows from the subsequent sections, the “electric” kilogram violates both these requirements while the “atomic” one respects them.

Thus we suggest the following criteria for choosing the optimal set of FPCs to be fixed for using in the new definitions of SI units:

A. Succession between the old and new definitions,
B. The stability requirement for transitions of the unit values,
C. A minimum number of FPCs to be fixed, the absence of new correction factors, and
D. A maximum simplicity of the relationship between a unit and the corresponding FPC, hence agreement between their dimensions.

4 Definitions of the kilogram and mole: the “electric kilogram” and related problems

By the time when the “light meter” was introduced (1983) and the value of the speed of light \( c \) was fixed, the conditions had been achieved for high-precision measurements of frequencies and the speed of light, exceeding by an order of magnitude or more the accuracy of length measurements. It was this circumstance that made it possible to fix the \( c \) value. For the four constants proposed to be fixed for redefinition of the SI units, viz., \( h, e, k, \) and \( N_A \), the present state of affairs is different, and for each of the constants there is a situation of its own. If one simultaneously adopts all new definitions of the SI units by fixing \( h, e, k \) and \( N_A \), this will lead, above all, to the problem of agreement between the values of these constants. Thus, fixing at once the values of \( h \) and \( N_A \), we would obtain a rigid connection between the speed of light in vacuum \( c \), the molar constant \( M_u \), the relative atomic mass of the electron \( A_r(e) \), the fine structure constant \( \alpha \) and the Rydberg constant \( R_\infty \) (see the relation (2.1)). To avoid such a connection, it is necessary to change the current definitions of these constants, e.g., the definition of the molar constant \( M_u \), and this is really suggested when introducing new definitions of the kilogram and the mole based on fixed values of \( h \) and \( N_A \) \[10\]. It is certainly a shortcoming of such new definitions because it transfers the molar constant \( M_u \) to the class of variable physical quantities \( (M_u = M_{u0}(1 + \kappa)) \), where \( \kappa \) is a correction to be determined from experimental data, and its value will change as new data emerge. This shortcoming can be avoided by introducing a definition of the kilogram on the basis of fixed values of the Avogadro constant and the atomic mass unit \[56\,57\] (see Section 5).

Besides, a definition of the kilogram based on a fixed value of \( h \) (the “electric kilogram” \[58\]) does not satisfy the succession criterion A (which would suggest to replace the IPK with a new standard having the dimension of mass), and there is no correspondence between the dimensions of a measurement unit and the related FPC (criterion D).

As to the stability requirement (criterion B), one can note that taking into account such external factors as microseisms, variable electromagnetic fields, the dependence of the gravitational
force on the place of measurement, etc., on the operation of a watt balance, it is very hard to satisfy this requirement at transfers of the value of the new kilogram using these complicated electromechanical devices. This inference is confirmed by the comparatively large systematic errors which had not been taken into account in the NIST experiment of 2007 [32].

We have to conclude that the “electric kilogram” does not satisfy any of the four criteria A–D formulated above for an optimal choice of constants with fixed values.

5 Definitions of the kilogram and mole: the “atomic kilogram” and its advantages

Let us consider in more detail the alternative redefinition procedure for the units of mass and the amount of substance in terms of fixed values of the Avogadro constant $N^*_A$ and the mass of a carbon-12 atom, or the atomic mass unit. In doing so, in order to respect the succession with the current SI, we suggest to preserve the definition of the molar mass of carbon-12, equal to 12 g. We thus satisfy the succession criterion and the criterion (3.1) on the dimensions of the measurement unit and the corresponding FPC, which role is now performed by the atomic mass unit. This procedure simultaneously specifies the microscopic mass standard on the basis of the carbon mass and the macroscopic mass standard on the basis of two invariants: the mass of a carbon atom and the fixed value of $N_A$. Let us note that the mass of a carbon atom is exactly fixed in the new mass unit after fixing the Avogadro constant. We thus suggest that the following relation should hold between the fixed numbers $N^*_A$ and $N^*_\text{kg}$:

$$N^*_A = 0.012 N^*_\text{kg},$$

where the fixed number of carbon atoms $N^*_\text{kg}$ specifies the macroscopic mass unit of the new SI, the kilogram*, and in this case the value of the molar constant $M_u$ related to the new units, kilogram* and mole*, will remain as it currently is [56, 57].

A new definition of the unit of mass can be formulated as follows:

*The kilogram*, a unit of mass, is the exact mass of $N^*_A/0.012$ free atoms of carbon-12 at rest, in the ground quantum state.

This definition corresponds to the following new definition of the mole:

*The mole*, a unit of the amount of substance, contains $N^*_A$ structure elements of this substance.

The suggested definitions of the kilogram and mole agree with the SI definitions of these units existing at present and preserve the existing connection between them. Consequently, in this case the existing values of the molar mass of carbon $M(^{12}\text{C})$ and the molar mass constant $M_{\text{rmu}}$, equal to 12 g/mole and 1 g/mole, respectively, are also preserved. At the same time, as is easily seen, the above definitions of the kilogram and mole can be adopted independently of each other.

To specify the value of $N^*_A$, one can use some additional conditions. Thus, it would be desirable that such widely used mass units of SI and CGS, the kilogram and the gram, contain a whole number of carbon-12 atoms. In this case the number $N^*_A$ should be a multiple of 12 [56]. And certainly, this value should belong to the experimentally determined range (1σ range) [34]:

$$N_A = (6.02214066 \div 6.02214102) \times 10^{23}.$$  

We thus obtain the following value of $N^*_A$:

$$N^*_A = 602214087869325727188096$$
and more concrete definitions of the kilogram and mole:

The kilogram is the unit of mass exactly equal to the mass of 5018450732243810599008 \times 10^3 free atoms of carbon-12 at rest, in the ground quantum state.

The mole is a unit of the amount of substance containing exactly 602214087860325727188000 structure elements of this substance.

These definitions of the kilogram and mole preserve a succession with the current SI definitions and do not violate the existing metrological chains of transferring the values of the units of mass and amount of substance as well as the existing practice of measuring masses, molar masses and amounts of substance [11, 18, 38, 59, 60].

As follows from the above-said, if this version is used for the definition of the kilogram, then a definition of the ampere based on a fixed elementary charge value should also become independent of other units and rest on the soon expected quantum standard. We believe it is also an important advantage: indeed, there is a nonzero probability that the metrological triangle will be closed not quite exactly, leading to certain corrections to the relations (2.3), which will in turn complicate the task of defining the ampere by fixing both \( h \) and \( e \).

Thus, in our view, the set of constants to be fixed connected with the “atomic kilogram” satisfies all the above four criteria A–D and is therefore preferable for the planned SI revision.

It should be noted for completeness that for the version of SI with the “atomic kilogram” we get for the Planck constant \( u_r(h) = u_r(N_A h) \), which is \( 0.7 \times 10^{-9} \) by CODATA-10. For the electric and magnetic constants \( \varepsilon_0 \) and \( \mu_0 \) obeying the relation \( \varepsilon_0 \mu_0 = 1/c^2 \), we get from the definition of the fine structure constant, \( \alpha = e^2/(2\varepsilon_0 hc) \), and Eq. (2.1)

\[
\begin{align*}
\mu_r(\varepsilon_0) &= \mu_r(\mu_0) = \mu_r(\alpha) = u_r(\varepsilon_0)/R_\infty, \\
\mu_r(\mu_0) &= \mu_r(\alpha) = u_r(\mu_0) = u_r(\alpha) = 10^{-9}
\end{align*}
\]

which is about \( 1 \times 10^{-9} \) according to CODATA-10. In the new SI version of [6] we have smaller values \( u_r(\varepsilon_0) = u_r(\mu_0) = u_r(\alpha) = 3.2 \times 10^{-10} \). But for the accuracies to be achieved in the new SI the value \( u_r(\varepsilon_0) = u_r(\mu_0) = 10^{-9} \) is sufficient.

6 Redefinition of the kelvin

By now, due to efforts of the international metrological organizations and national metrological institutes, the first problem of redefinition of the unit of thermodynamic temperature, the kelvin, can be considered as a solved one. That is, the kelvin should be defined by fixing the exact value of the Boltzmann constant.

This belief is connected with the nature of the Boltzmann constant as a conversion factor between two temperature scales [6, 61–63]. Indeed, the temperature enters into thermodynamic laws as the combination \( \theta = kT \) (according to Gibbs [61], the modulus of distribution), and it is this quantity that is measured in experiments.

It has been shown [64] that in a molecular system of finite size all thermodynamic functions are analytic functions of their variables and have no discontinuities even in phase transition domains. Mathematically, a transition from one phase to another in the space of thermodynamic parameters (e.g., temperature and pressure) occurs in a continuous manner, though in a very narrow domain of nonzero size. Moreover, the larger is the size of a molecular system, the more narrow is this transition domain in the thermodynamic parameter space. Only if the size of the molecular system tends to infinity, the size of the phase transition domain in the space of thermodynamical parameters tends to zero in the thermodynamic limit [64], and discontinuities emerge in the equation of state.
As to real macroscopic systems, it is, strictly speaking, impossible to specify for them the temperature of a phase transition or the temperature of coexistence of three phases (like the temperature of the triple point of water in the energetic scale, $\theta_{TPW}$) with zero uncertainty because the transition domain in the space of thermodynamical parameters has formally a nonzero size. Accordingly, the thermodynamic temperature $T_{TPW}$ cannot be specified with zero uncertainty. However, the coefficient that connects these two temperature scales can be specified exactly. It is this circumstance that underlies the suggested redefinition of the thermodynamic temperature unit.

Though, physically, the thermometric instruments have measurement uncertainties greater by many orders of magnitude than the size of the above phase transition domain for a real macroscopic system. Therefore, a thermometer perceives it as a single point of discontinuity, which is then called a phase transition point. One of such points, the triple point of water, is presently used for a definition of the kelvin, such that the exact value of its thermodynamic temperature is $T_{TPW} = 273.16$ K.

Measurements of the “energetic” temperature of the triple point of water $\theta_{TPW}$ by primary thermometers make it possible to find experimentally the Boltzmann constant value from the relation $k = \theta_{TPW}/273.16$. The accuracy of such experimental determination of $k$ is the same as the accuracy of measuring $\theta_{TPW}$. This value of $k$ is after that used in all measurements of the thermodynamic temperature, and its uncertainty contributes to the total uncertainty of the measured thermodynamic temperature.

It is clear that fixing the exact value of the Boltzmann constant better corresponds physically to the ideas of modern statistical mechanics than fixing the exact value of the temperature of a particular phase transition in one of the temperature scales [13, 63, 65].

The second task for introducing a new definition of the kelvin is finding the exact value of the Boltzmann constant. The most direct method of determining the $\theta_{TPW}$ value is its theoretical calculation in the framework of statistical mechanics [13, 63, 65]. However, by now, not only methods of its exact calculation are absent, but there is even no method of its approximate calculation with the accuracy achieved in measuring $k$ in modern gas thermometers of various types. Therefore, the most real way is the experimental determination of the Boltzmann constant with the required accuracy. As shown in Section 2, this problem is being solved successfully, and it looks quite probable that in the nearest three or four years the values of the Boltzmann constant will be obtained in a few independent laboratories with an accuracy sufficient for making a transition to a new definition of the kelvin.

So there is a substantial difference in the state of affairs with redefinition of the kelvin and that with the units of mass and amount of substance. Consequently, as soon as the value of $k$ is measured with the necessary accuracy, $u_k = 1 \times 10^{-6}$, one can introduce a new definition of the kelvin irrespective of whether the necessary accuracies of measuring $h$, $N_A$ and $e$ will be achieved by that time.

7 Conclusion

We have analyzed the suggested versions of new definitions of the kilogram, ampere, kelvin and mole based on fixing the exact values of certain FPCs, and formulated some criteria for choosing the set of FPCs with fixed values suitable for redefinition of the base SI units. These include (A) succession between the new and old definitions, (B) stability in transferring the value of a unit, (C) a minimum number of FPCs fixed and absence of new correction factors, and (D) agreement in
dimensions of the base unit and the corresponding FPC. In particular, these criteria are satisfied by the mass of carbon-12 and the electron’s electric charge. We have demonstrated the advantages of a new definition of the kilogram on the basis of the atomic mass unit (the “atomic kilogram”), at which the molar mass of the carbon isotope $^{12}$C, equal to 12 g/mole, will be preserved.

Fixing the atomic mass unit and the Avogadro constant $N_A$ would lead to quite clear and logically perfect definitions of the kilogram and mole, compatible with the definitions of these two units being in force at present, and with the current practice of measurements of mass, molar mass and amount of substance [42, 56]. Besides, the fixed values of the mass of a carbon-12 atom and the Avogadro constant are natural invariants. We can note that in 2011 the Commission on Relative Isotope Content and Atomic Weights (CIAAW) of the International Union of Pure and Applied Chemistry (IUPAC) has supported the definition of the kilogram based on the atomic mass unit (dalton) [43].

It is known that while the basic physical quantities used in metrology are assumed to be independent of each other, for the corresponding measurement units such a dependence is still admissible. For instance, in the current SI the definition of the mole depends on that of the kilogram, and the mole can only be defined after defining the kilogram. However, as we saw in Section 5, it is possible to make the units of mass and the amount of substance mutually independent and equal in rights but still preserve the existing relationship between them.

The “electric kilogram” concept, implying a fixed value of the Planck constant $h$, not only violates the four criteria described above, but also leads to certain difficulties in defining the ampere. The $h$ value being fixed, the ampere is redefined by fixing also the electron charge $e$, hence the quantities $2e/h$ and $h/e^2$ will take exact values, and the practical electric units $Ω_{90}$ and $V_{90}$ will belong to the class of units of the new SI, which is favourable for the metrology of electric measurements. However, as argued above, this cannot be realized until the quantum metrological triangle is closed, and it can happen that it will not be closed quite exactly. Therefore there are serious reasons to attribute the Planck constant to the class of electromagnetic quantum constants (as suggested in the “atomic kilogram” concept), together with the Josephson ($K_J$) and von Klitzing ($R_K$) constants. Then a new definition of the ampere will be provided by a new quantum standard on the basis of single-electron tunneling and a fixed value of $e$ only and will not depend on the definition of the kilogram and the value of $h$. In this case, the values of $K_J$ and $R_K$ will be found by reconciling the results of various experiments with the same or better accuracy than the current one. The practice of using fixed values of $K_J$ and $R_K$ can be preserved at a certain accuracy level, leaving open the opportunity of measuring $h$ more and more accurately for testing the existing theories and a search for new ones.

Thus the new SI version with the “atomic kilogram” makes all the four units in question mutually independent.

Concerning the kelvin, as follows from the discussion in Section 6, it is physically more preferable to define it by fixing an exact value of the Boltzmann constant as a conversion factor between two temperature scales than by fixing the temperature of the triple point of water in one of the temperature scales (the thermodynamic one).

The most accurate values of the Boltzmann constant have been obtained by acoustic gas thermometers. Other methods are so far less accurate. All experimental results require a thorough analysis of the total uncertainty budget, including an accuracy estimate of the equation of state of the working substance and confirmation in independent experiments using different types of equipment. The current dynamics of accuracy increase of the methods and means of primary thermometry shows that a reliable achievement of the required measurement uncertainty $u_r(k)$
of the Boltzmann constant by the time of the 26th CGPM is quite a real task. As soon as this accuracy is achieved, it will be possible to introduce a new definition of the kelvin irrespective of whether or not there are necessary conditions for introducing new definitions of the kilogram, mole and ampere.

The new SI adoption is now planned to occur at the CGPM in 2018 [9]. There is so far enough time to consider the advantages and shortcomings of the suggested new definitions of the SI units and their different versions (see, e.g., [43–45]) taking into account the fulfilment of all necessary criteria and further progress in reducing the relative uncertainties of the relevant FPC measurements, with a hope that there will be the same improvement as at the introduction of the new metre in 1983.

Abbreviations

BIPM — Bureau International des Poids et Mesures.
INRiM — Istituto Nazionale di Ricerca Metrologica, Italy.
LNE-CNAM, France:
  LNE — Laboratoire National de métrologie et d’Essais,
  CNAM — Conservatoire national des arts et métiers.
NIST — National Institute of Standards and Technology, USA.
NMIJ — National Metrology Institute of Japan.
NPL — National Physical Laboratory, United Kingdom.
NRC — National Research Council, Canada.
PTB — Physikalisch-Technische Bundesanstalt, Germany.

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