The Kilogram in the "New SI"

For good reason, chemists regularly follow progress made by the Bureau International des Poids et Mesures (BIPM) toward the so-called "New SI." The International Committee for Weights and Measures (CIPM) of the BIPM continues to ponder over the redefinition of the kilogram, which is the only base unit of the SI still tied to an artifact. CIPM drafted a Resolution for consideration this coming October at the General Conference on Weights and Measures (CGPM) meeting, noting its intention to redefine four of the SI base units, namely the kilogram, the ampere, the kelvin, and the mole, in terms of invariants of nature. The new definitions would be based on fixed numerical values of the Planck constant (h), the elementary charge (e), the Boltzmann constant (k), and the Avogadro constant (N_A), respectively. In order to encourage communication, awareness, and debate on the possible revision of the SI, BIPM has provided key draft documents on its website at www.bipm.org/en/si/new_si.

Readers of *CI* have been informed of these developments and in several instances Ian Mills, IUPAC representative on CIPM Consultative Committee on Units (CCU) and president of CCU, has reviewed the issues; see "An Update on the Kilogram" (*CI* Sep-Oct 2005, pp. 12-15); "Amount and Substance and the Mole," I. Mills and M. Milton (*CI* Mar-Apr 2009, pp. 3-7); "What is a Mole? Old Concepts and New" by Jack Lorimer, "A Fixed Avogadro Constant or a Fixed Carbon-12 Molar Mass: Which One to Choose? by Y. Jeannin, and "Closing Comment" by Ian Mills (*CI* Jan-Feb 2010, pp. 6-11)

In this two-part feature, Albert C. Censullo et al. start with a review of the status of the kilogram and their understanding of it and end by offering an alternative proposal. In part II, Ian Mills responds by reviewing the rationale behind the proposed new SI, the concept of explicit-constant definitions, and the implications of the definitions of both the kilogram and mole.



The kilogram, kept by the Bureau International des Poids et Mesures.

Part I—From the Current "Kilogram Problem" to a Proposed Definition

by Albert C. Censullo, Theodore P. Hill, and Jack Miller

he metric system of measurements has served the international scientific and technical communities well since its inception over 200 years ago. By the mid 1800s, three so-called "base units" were in place, for measuring distance, mass, and time (centimetre, gram, second, or CGS system). These base units evolved into the metre, kilogram, and second (MKS system). The ampere became the fourth base unit in 1946. In 1954, the kelvin and candela became new base units. Finally, in 1971, the mole became the seventh base unit, for amount of substance. The definitions of each base unit have undergone continuous evolution, corresponding to improvements in measuring capabilities, and recognition of shortcomings of prior definitions. As stated by BIPM, "The SI is not static but evolves to match the world's increasingly demanding requirements for measurement."

Of the seven base units in existence today, only one of them is based on a physical artifact. The current definition for the kilogram is embodied in Le Grand K, the platinum-iridium cylinder maintained by the BIPM in Sèvres, near Paris. Comparisons with virtually identical artifacts suggest that the mass of Le Grand K may have changed by 50 micrograms, or possibly even more, from its date of creation in 1884. Starting with the 1963 redefinition of the second and the 1983 redefinition of the metre, there has been a call to replace the definition of the kilogram with a more suitable one, using some "invariant of nature" to replace the artifact kilogram.¹ Since the perceived weakness of the current SI definitions of other units such as the ampere, mole, and candela "derives in large part from their dependence on the kilogram . . . the definition of the kilogram is thus central to the more general problem of improving the SI."² This so-called "kilogram problem" is the subject of this paper.

Current Proposed Definition for the Kilogram

Following the success of the redefinition of the second and the metre, a revision of the entire system of measurements was envisioned, based on defining units based on fundamental constants. As stated in the current draft *SI Brochure* for the proposed new SI,³ "The present definitions of the seven base units are made in terms of the values of seven fundamental constants that are believed to be true invariants throughout time and space, available to anyone, anywhere, at any time, who wishes to realize and make use of the values of the units to make measurements."

Effort was made to maintain style consistency in the new definitions. The proposed definitions belong to a class known as "explicit-constant definitions." In the draft proposal, each definition is linked to a specific fundamental constant and states explicitly the numerical value of the fixed constant. Underlying principles and laws of physics are intended to allow the definition of the unit to become apparent. According to BIPM,1 "The metre is the length of the path travelled by light in vacuum during a time interval of 1/299 792 458 of a second." In that case, the relationship between speed, time, and distance is obvious, and easily comprehended. As will be seen, this is not quite the case for the new kilogram definition.

A set of preliminary proposals under consideration by BIPM for redefining the kilogram began appearing in the literature five or six years ago.^{2,4} The idea put forth involved the establishment of either an "electronic kilogram" or an "atomic kilogram," whose definition would be based on fixing the value of either of two constants, Planck's constant or Avogadro's constant, respectively. Eventually, redefinition via Planck's constant, the electronic kilogram, became the recommended approach by the Consultative Committee on Units and it was forwarded on to the BIPM. This has been verified by the BIPM's release of the draft chapter 2 of the 9th edition of the *SI Brochure* in which the proposed new definition for the kilogram is as follows:

"The kilogram, kg, is the unit of mass; its magnitude is set by fixing the numerical value of the Planck constant to be equal to exactly 6.626 06 X x 10^{-34} when it is expressed in the unit s⁻¹ m² kg, which is equal to J s."

(The "X" refers to as-yet-unspecified additional digits.)

The indirect implied relationship between the kilo-

gram and Planck's constant is not immediately apparent from the definition, and requires knowledge of both special relativity and quantum mechanics.^{5,6}

Mills et al.² present a case for dramatic changes to the SI system of units. They noted that the most important quality of newly defined units was that the defining quantity should be a true invariant of nature. The International Committee for Weights and Measures of the BIPM called for the widest possible publicity be given to these ideas among the scientific and user communities (94th meeting in October 2005). Other important factors were as follows: (a) practical realization of definition should be possible anywhere, at anytime; (b) definition should be readily comprehensible to students in all disciplines; and (c) continuity of definition should be preserved, for consistency with older definition.

Criticism of the Proposed SI

In the past year or two, there has been increasing discussion appearing in the literature by members of the international scientific community on the proposed system referred to by BIPM as the "New SI."

The Consultative Committee on Units' recommendation, which IUPAC supports, is to define the mole as the amount of substance of specified elementary entity, such that the Avogadro constant is exactly $6.022 \ 141 \ 79 \times 10^{23}$ per mole.² This means that a mole contains Avogadro's number of entities. The result of this assignment is that the molar mass of ¹²C will no longer be fixed by definition, but will be an experimental quantity.

Leonard⁷ points out a "compatibility condition" that naturally exists between Planck's constant, Avogadro's constant, and the mass of the carbon-12 atom, such that $h N_A = K_c M(^{12}C)$, where K_c is a combination of constants: $K_c = (c_o/2)(1/R_{\infty})[m_e/m(^{12}C)]\alpha^2$. He points out that any two of the quantities (h, N_A , $M(^{12}C)$) may be fixed, but the third must be related by the aforementioned compatibility condition. If we wish to maintain $M(^{12}C)$ as exactly 12, either h or N_A must be determined experimentally; they cannot both be assigned exact values. If both h and N_A are fixed (as in the proposed New SI definition), the mass of the carbon-12 atom will no longer be fixed, but becomes a quantity to be determined (and re-determined) experimentally, as higher precision techniques may eventually allow. This variance of what chemists normally consider invariant causes its own "kilogram problem."

<u>Part I</u>

Dissenting from the CCU view, Jeannin⁸ noted the present definition of the mole (amount of substance containing as many entities as there are atoms in 0.012 kg of carbon-12) implies a fixed molar mass of carbon-12 $M(^{12}C)$ as exactly 12 grams/mole. This definition requires that the unit of mass (kilogram) must be defined prior to defining the mole. The proposed definition² de-couples the mole from the kilogram, which was viewed as desirable. However, the three values for Planck's constant (h), the Avogadro constant (N_A), and carbon-12 molar mass, $M(^{12}C)$, are still linked. This presents a dilemma to the chemist, who tends to think of the carbon-12 atom as a "true invariant of nature," perhaps the ultimate invariant of nature.

Khruschov⁶ compares defining the kilogram in terms of either h or N_A . He describes the watt-balance method for producing an "electronic kilogram," based on the equation relating electrical and mechanical power that may be written as mgu/K = h/4. By fixing the value for h, the mass may be "measured," based on other known constants and experimental variables (velocity, voltage, and current) which have very small uncertainties. He states, "the basis of this definition will not be a natural invariant, such as the mass of a carbon atom, but an artificially created electromechanical device, the watt balance, with a large number of sources of systematic uncertainty."6 As of this date, discrepancies between experimental values for Planck's constant determined by U.S. and U.K. watt balance teams have not been resolved.

The alternative "atomic kilogram" is based on an exact value for Avogadro's number, so an accurate count of a large number of atoms must be made. The current method for obtaining this number is based on a crystalline silicon sphere, and complications of this experiment include uncertainties in isotopic abundance of the silicon atoms, as well as impurities and defects in the crystal, and adsorbed surface oxides. Khruschov and his colleagues find an atomic kilogram "logically consistent and intuitive, which makes it convenient for use in education." They propose the definition: the kilogram is the exact mass of $N_{\rm A}/0.012$ free atoms of carbon-12, where N_A must be a multiple of 12 so that the gram and kilogram will contain an integral number of atoms. They conclude "new definitions of the units of mass and amount of substance should be based on a fixed value of the Avogadro constant⁹ and the mass of the carbon atom." We share this view.⁵

Milton et al. outlined several key aspects desired in an updated SI system.¹⁰ They recognized the need for a dynamic measuring system, responsive to scientific and technological advances, that is responsive to the needs and views of the scientific community of users. As stated in that article, "Any new definition must be comprehensible to this audience . . ." The New SI System's reliance on guantum standards, intended to reduce the uncertainty in measurements, limits the realization of the definitions to highly specialized experimentations with equipment that is not readily available. For example, to realize the new definition of the kilogram, a watt balance is often suggested as the mise en pratique. There are only a few of these expensive and complex devices in the global metrology community. This hardly fulfills the BIPM directive that "The new definitions will be referenced to true invariants of nature, and may be realized by anyone, anywhere, at any time."1 Milton et al. find that the redefinition of the kilogram is premature, and potentially dangerous to the integrity of the SI System. Their [2007] conclusion, "At present, there is insufficient experimental evidence to justify any proposed resolution of the 'kilogram problem' . . ." should serve as a caution to those interested in any potential immediate redefinition of the kilogram.

A number of issues concerning the "New SI" have been raised in the summary article by G. Price.¹¹ Some objections include: difficulty in explaining definitions to new users of the SI system (including beginning students in the physical sciences); continued use (rather than clarification) of the confusing term "amount of substance"; increasing interdependency of base units (making systematic errors more difficult to detect, and complicating the redefinition of any single unit); likely inconsistencies produced by fixing the exact values of many physical "constants" (unless the exact "correct" values for all of these constants happened to be fortuitously chosen). The author refers to the new kilogram definition in this way: "the most obvious source of confusion in the New SI will be the definition of the kilogram, which no longer makes any reference to any real mass of any kind, artifactual or natural."

A Constructive Alternative

As an alternative to the proposed electronic kilogram, a concrete atomic kilogram has been described.⁵ There, some of the perceived shortcomings associated with the proposed New SI definition are described in detail. In lieu of that definition, an alternate formulation based on fixing Avogadro's constant is proposed, which is pedagogically simpler, and is based on a true

The Kilogram in the "New SI"

invariant of nature, the carbon-12 atom. Under this definition,

"a kilogram is the mass of 84 446 8893 x 1000/12 unbound atoms of carbon-12 at rest, in their ground state."

The factor of 1000 is, of course, a necessary requirement that results from the use of the kilogram (rather than the gram) as the unit of mass. This definition fully satisfies the desirable qualities of unit redefinition, (a), (b), (c) above. It has the added advantage of maintaining the value of the carbon-12 atom at its exact value of 12, ensuring that tables of atomic masses will not need to be periodically adjusted.

We hope that the scientific community has adequate opportunity to review and propose alternative definitions for the kilogram, as well as other SI units, before any changes are promulgated. A delay in producing a "New SI" seems to be a perfectly acceptable alternative for the present.

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Part II—Explicit-Constant Definitions for the Kilogram and for the Mole

by Ian Mills

Censullo et al. suggest the following changes to the present proposals for the new SI. They prefer explicitunit definitions over the proposed explicit-constant definitions of all the units. They would prefer the kilogram to be redefined to fix the mass of an atom. such as the carbon 12. rather than to fix the value of the Planck constant. They would prefer the mole, and hence the Avogadro constant, to be defined to fix the molar mass of carbon 12 (which is the current definition) rather than by defining the mole explicitly by specifying the number of entities in a mole, and thus fixing the numerical value of the Avogadro constant. Each of these issues is discussed in turn below. A more detailed discussion can be found in reference 1. The copy of Resolution A for the 24th CGPM to be held in October 2011,² and the FAQs,³ are also relevant; both are available on the BIPM website.

Explicit-constant versus explicit-unit definitions

The distinction between explicit-unit and explicitconstant definitions may be illustrated by the present definition of the metre. The more familiar explicit-unit definition reads:

The metre is the length of path travelled by light in vacuum in 1/299 792 458 of a second.

Exactly the same definition expressed in the proposed explicit-constant form reads:

The metre, m, is the SI unit of length; its magnitude is set by fixing the numerical value of the speed of light in vacuum to be equal to exactly 299 792 458 when it is expressed in the unit m s⁻¹.

The advantage of the explicit-constant format is that it emphasizes the reference constant used in the defini-