

# Mise en pratique of the definition of the kilogram

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## Consultative Committee for Mass and Related Quantities (CCM) Working Group on the Realization of the Kilogram (WGR-kg)

(*Editor's note 0.1:* In the following text, all digits in red are meant to be place holders for the final digits to be inserted at the time of approval of the redefinition.)

### 1. Introduction

#### 1.1 Definition of the kilogram

The kilogram, the unit of mass in the International System of Units, SI, is defined in Resolution XX adopted by the XXth CGPM in 20XX [1.1]. It reads:

**The kilogram, symbol kg, is the SI unit of mass; its magnitude is set by fixing the numerical value of the Planck constant to be exactly  $6.626\ 069\text{X} \times 10^{-34}$  when it is expressed in the SI unit for action  $\text{J s} = \text{kg m}^2 \text{s}^{-1}$ .**

Thus the Planck constant,  $h$ , is exactly  $h = 6.626\ 069\text{X} \times 10^{-34}$  J s. This numerical value of  $h$  defines the magnitude of J s in the SI and, in combination with the SI second and metre, defines the magnitude of kg in the SI. The numerical value of  $h$  thereby ensures the continuity of the unit of mass with the previous definition, as explained in section 4.

The value of  $h$  is that recommended by the CODATA Task Group on Fundamental Constants based on experimental results that were available prior to the cut-off date of XXXXX [1.2]. Under conditions presented in section 2, the kinds of experiments which determined  $h$  have the potential to become primary reference measurement procedures (referred to as “primary methods” in this document) to realize the new definition based on the numerical value for  $h$  that is fixed in the definition of the kilogram cited above.

#### 1.2 Traceability chain for mass metrology

The definition of the unit of mass does not imply or suggest any particular experiment to realize it. This document recommends primary methods of practical realization of the mass unit. A primary method is a method for determining a mass in terms of  $h$  without use of a mass standard (Figure 1).

The mass whose value is to be determined may be an artefact, atom or other entity although the following focuses on metrology for mass artefacts at the highest level of accuracy. Such an artefact whose mass has been directly calibrated by a primary method to realize the kilogram definition becomes a primary mass standard. Secondary mass standards are established through calibration with respect to primary mass standards.

This document focuses on the realization and dissemination of the unit of mass at a nominal value of 1 kg. The *mise en pratique* may be updated to include information on primary methods at different nominal mass values.

Primary methods for the realization of the definition of the kilogram and procedures for its dissemination through primary mass standards are described in the following two sections. The traceability chain is shown schematically in Figure 1.

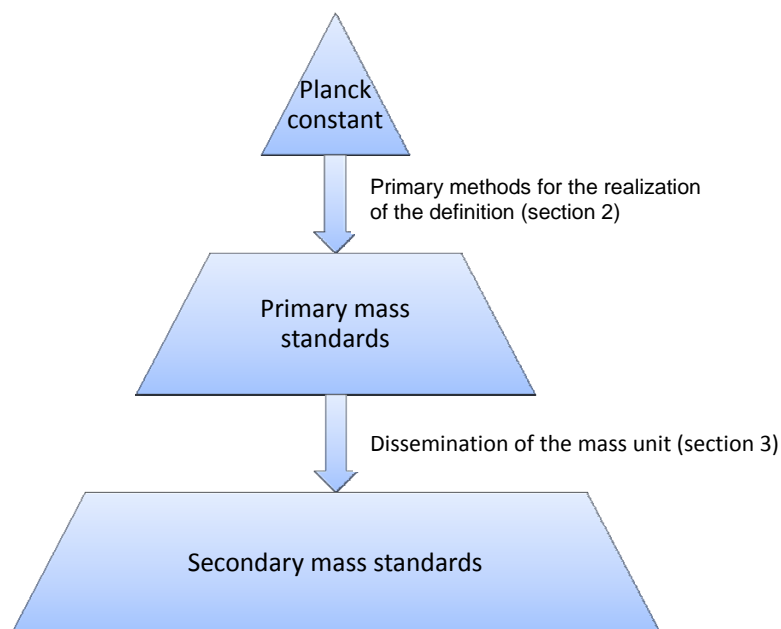


Figure 1. Illustration of the traceability chain from the definition of the kilogram to primary and secondary mass standards. The unit of the Planck constant being  $\text{kg m}^2 \text{s}^{-1}$ , the units second and metre are needed to derive a primary mass standard from the Planck constant.

This *mise en pratique* will be updated to take account of new methods and technological improvements. It is not printed in the *SI Brochure* [1.1], but the current version is posted on the open BIPM web site at [http://www.bipm.org/en/si/si\\_brochure/appendix2/](http://www.bipm.org/en/si/si_brochure/appendix2/).

## 2. Primary methods to realize the definition of the kilogram

There are currently two independent primary methods that are capable of realizing the definition of the kilogram with relative uncertainties within a few parts in  $10^8$ . The first of these relies on determining the unknown mass using an electromechanical balance specially designed for the purpose. The second method compares the unknown mass to the mass of a single atom of a specified isotope, where the latter is well-known in terms of  $h$ .

### 2.1 Realization by comparing electrical power to mechanical power

Accurate instruments that function in a way that electrical and mechanical power can be equated are known as watt balances. Watt balances can be designed with different geometries and experimental protocols. The following schematic description serves to demonstrate that any of these watt-balance configurations has the potential to be a primary method to realize the definition of the kilogram.

The determination of the unknown mass  $m_x$  of an artefact  $x$  is carried out in two modes: the weighing mode and the moving mode. They may occur successively or simultaneously. In the weighing mode, the weight<sup>1</sup>  $m_x g$  of the artefact is balanced by the electromagnetic force produced, for example, on a circular coil of wire-length  $l$  immersed in a radial magnetic field of flux density  $B$  when a current  $I_1$  flows through the coil. The magnet and coil geometries are designed to produce a force that is parallel to the local gravitational acceleration. The acceleration of gravity  $g$  acting on the mass, and the current  $I_1$  flowing in the coil are measured simultaneously so that

$$m_x g = I_1 B l. \quad (2.1)$$

In the moving mode the voltage  $U_2$ , which is induced across the terminals of the same coil moving vertically at a velocity  $v$  through the same magnetic flux density, is measured so that

$$U_2 = v B l. \quad (2.2)$$

The equations describing the two modes are combined by eliminating  $B l$ :

$$m_x g v = I_1 U_2. \quad (2.3)$$

Thus power of a mechanical nature is equated to power of an electromagnetic nature. The powers are manifestly “virtual” in this method of operation because power does not figure in either mode of this two-mode experiment.

The current  $I_1$  can, for example, be determined using Ohm’s law by measuring the voltage drop  $U_1$  across the terminals of a stable resistor of value  $R$ . Both voltages,  $U_1$  and  $U_2$ , are measured in terms of the Josephson constant,  $K_J$ , which  $K_J$  is taken to be  $K_J = 2e/h$ ;  $e$  is the elementary charge. Similarly,  $R$  can be measured in terms of the von Klitzing constant  $R_K$  which is taken to be  $R_K = h/e^2$ . The quantities  $v$  and  $g$  are measured in their respective SI units,  $\text{m s}^{-1}$  and  $\text{m s}^{-2}$ . Note that  $K_J^2 R_K = 4/h$  allowing (2.3) to be rewritten schematically as

$$m_x = h \left( \frac{b f^2}{4} \right) \frac{1}{g v}, \quad (2.4)$$

where  $f$  is an experimental frequency and  $b$  is a dimensionless experimental quantity, both associated with the required measurements of electrical current and voltage [2.2].

All relevant influences on the mass,  $m_x$ , as derived from (2.4) must be considered for the realization, maintenance and dissemination of the unit of mass (see also Annex A3).

Other electromagnetic and electrostatic realizations have been proposed, such as the joule-balance and volt-balance methods, and may well be perfected [2.3].

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<sup>1</sup> In legal metrology “weight” can refer to a material object or to a gravitational force. The terms “weight force” and “weight piece” are used in legal metrology if the meaning of “weight” is not clear from the context [2.1].

## 2.2 Realization by the X-ray-crystal-density method

The concept of the X-ray-crystal-density (XRCD) method comes from a classical idea where the mass of a pure substance can be expressed in terms of the number of elementary entities in the substance<sup>2</sup>. Such a number can be measured by the XRCD method in which the volumes of the unit cell and of a nearly perfect crystal are determined, e. g. by measuring the lattice parameter  $a$  and the mean diameter of a spherical sample. Single crystals of silicon are most often used in this method because large crystals can be obtained having high chemical purity and no dislocations. This is achieved using the crystal growth technologies developed for semiconductor industry. The macroscopic volume  $V_s$  of a crystal is equal to the mean microscopic volume per atom in the unit cell multiplied by the number of atoms in the crystal. For the following, assume that the crystal contains only the isotope  $^{28}\text{Si}$ . The number  $N$  of atoms in the macroscopic crystal is therefore given by

$$N = 8V_s/a(^{28}\text{Si})^3, \quad (2.5)$$

where 8 is the number of atoms per unit cell of crystalline silicon and  $a(^{28}\text{Si})^3$  is the volume of the unit cell, which is a cube; i.e.,  $V_s/a(^{28}\text{Si})^3$  is the number of unit cells in the crystal and each unit cell contains eight silicon-28 atoms. Since the volume of any solid is a function of temperature and, to a lesser extent, hydrostatic pressure,  $V_s$  and  $a(^{28}\text{Si})^3$  are referred to the same reference conditions. For practical reasons, the crystal is fashioned into a sphere having a mass of approximately 1 kg.

To realize the definition of the kilogram, the mass  $m_s$  of the sphere is first expressed in terms of the mass of a single atom, using the XRCD method<sup>3</sup>:

$$m_s = N m(^{28}\text{Si}), \quad (2.6)$$

Since the experimental value of the physical constant  $h/m(^{28}\text{Si})$  is known to high accuracy [2.4], one can rewrite (2.6) as

$$m_s = h N \left( \frac{m(^{28}\text{Si})}{h} \right). \quad (2.7)$$

The XRCD experiment determines  $N$ ;  $m(^{28}\text{Si})/h$  is a constant of nature whose value is known to high accuracy and, of course, the numerical value of  $h$  is now exactly defined.

The sphere is a primary mass standard and the unit of mass, the kilogram, is

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<sup>2</sup> The measurements described here were first used to determine the value of the Avogadro constant  $N_A$ , which is defined as the number of elementary entities in one mole of substance. An accurate measurement of  $N_A$  was an essential contribution on the road to redefining the kilogram in 20XX. Today, however, the numerical value of  $N_A$  is exactly defined when expressed in the SI unit  $\text{mol}^{-1}$  thus making the definition of the mole independent of the kilogram.

<sup>3</sup> It is well known that (2.6) is not exact because the right-hand side is reduced by the mass equivalent,  $E/c^2$ , of the total binding energy  $E$  of the atoms in the crystal, where  $c$  is the speed of light in vacuum. The correction, about 2 parts in  $10^{10}$ , is insignificant compared with present experimental uncertainties and has been ignored. Additional energy terms (e.g. thermal energy) are even smaller than the binding energy and thus negligible.

disseminated from this standard. Spheres currently used in this work are enriched in the isotope  $^{28}\text{Si}$  but the presence of trace amounts of two additional silicon isotopes leads to obvious modifications of the simple equations presented in this section. See [2.5] for a more complete analysis of this experiment.

All relevant influences on the mass of the sphere,  $m_s$ , as derived from (2.7) must be considered for the realization, maintenance and dissemination of the unit of mass (see also Annex A3).

### **3. Dissemination of the mass unit**

The definition of the kilogram ensures that the unit of mass is constant in time and that the definition can be realized by any laboratory, or collaboration of laboratories, with the means to do so. Any NMI, DI, the BIPM, or collaboration among them, that realizes the kilogram definition can disseminate the SI kilogram from its primary mass standards to any other laboratory or, more generally, to any user of secondary mass standards (see Figure 1). This is described in section 3.1.<sup>4</sup> Dissemination from a dedicated ensemble of 1 kg secondary standards maintained at the BIPM, called BIPM ensemble of reference mass standards, is described in section 3.2.

#### *3.1 Dissemination from a particular realization of the kilogram*

The dissemination of the mass unit is based on primary mass standards obtained from the realization of the definition of the kilogram according to the methods described in section 2. All relevant influences on a primary mass standard must be considered for the maintenance and dissemination of the mass unit (see Annex A3). In particular, the uncertainty due to a possible drift of the primary mass standards since the last realization must be taken into account.

The BIPM in coordination with the CCM organizes an on-going BIPM key comparison [3.1], BIPM.M-K1 [3.2], for laboratories with primary realization methods. In this comparison, the primary mass standards of the participants are compared to artefacts from the BIPM ensemble of reference mass standards (see section 3.2). The CCM decides the required periodicity of laboratory participation in BIPM.M-K1 in order to support relevant calibration and measurement capabilities (CMCs).

In cases where compliance with the CIPM MRA is required [3.3], it is essential that the mass standards are traceable to primary mass standards of a participant in BIPM.M-K1 that has relevant CMC entries or, in the case of the BIPM, suitable entries in its calibration and measurement services as approved by the CIPM. Dissemination of the whole mass scale is validated for all NMIs/DIs and the BIPM through the traditional types of key comparisons organized prior to the present definition of the kilogram.

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<sup>4</sup> Experience teaches that statistically significant differences are sometimes observed between independent measurements or realizations of a unit. In rare cases such differences are unacceptable to the user. In order to attain and to preserve a high degree of international equivalence in the dissemination of the kilogram, generally accepted methods and procedures are described in section 3 and Appendix 4.

Results of all key comparisons are published in the Key Comparison Database (KCDB) in accordance with the rules of CIPM MRA [3.1] and may be used in support of NMI/DI claims of its calibration and measurement capabilities (CMCs) and the BIPM claims listed in its calibration and measurement services.

### *3.2 Dissemination from the BIPM ensemble of reference mass standards*

In accordance with Resolution 1 of the 24<sup>th</sup> meeting of the CGPM (2011), the BIPM maintains an ensemble of reference mass standards “*to facilitate the dissemination of the unit of mass when redefined*” [3.4].

This ensemble is presently composed of twelve 1 kg artefacts of various materials which have been chosen to minimize known or suspected sources of mass instability. A storage facility has been designed to minimize the rate of surface contamination of the artefacts. Technical details are provided in [3.5].

The average mass of the ensemble is derived from links to primary realizations of the kilogram definition that have participated in an initial pilot study and in BIPM.M-K1 through an algorithm given in the key comparison protocol. The BIPM<sup>5</sup> disseminates the unit of mass from the average mass of the ensemble. NMIs, DIs, the BIPM or collaborations among them, may adopt a similar strategy for dissemination of the mass unit.

## **4. Continuity with the previous definition of the kilogram**

Preserving the continuity of measurements traceable to an SI unit before and after its redefinition is a generally accepted criterion for revised definitions of SI base units. The previous definition of the kilogram was based on the mass of the international prototype of the kilogram (IPK) immediately after the prescribed cleaning procedure. The dissemination of the mass unit therefore required traceability to the mass of the IPK.

Prior to the adoption of Resolution **XX** of the **XX**th CGPM (20**XX**), all mass standards used for the experimental determination of the Planck constant were calibrated by an “extraordinary use” of the IPK [4.1]. Additionally the BIPM ensemble of reference mass standards was calibrated.

A pilot study was performed to prepare for the redefinition of the kilogram [4.2]. The comparison included all available experiments capable of determining the value of the Planck constant to high accuracy. Measurements were made over a period of less than **XX** months.

By agreement of the CGPM, the CODATA Task Group on Fundamental Constants evaluated all published experimental values for the Planck constant  $h$  and recommended the numerical value of  $h$  to be used for the new definition of the

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<sup>5</sup> The BIPM operates under a quality management system (QMS) that conforms to ISO/IEC 17025:2005. The QMS is under the exclusive supervision of the CIPM. Competence is demonstrated through on-site audits conducted by external experts and regular reports to CIPM Consultative Committees and Regional Metrology Organizations.

kilogram [1.2]. The Task Group also recommended the relative uncertainty of  $h$ , which was assigned to the international prototype of the kilogram just after fixing the numerical value of  $h$ . As a consequence, just after the redefinition, the mass of the IPK was still 1 kg, but within an uncertainty of  $x$  parts in  $10^{-8}$ . Accordingly, all mass values traceable to the IPK were unchanged when the new definition came into effect, but all associated uncertainties of these mass values were increased by a common component of relative uncertainty, equal to the relative uncertainty of the IPK just after the redefinition.

When the unit of mass is realized according to 2.1 or 2.2, the uncertainty budgets of all mass standards traceable to this realization contain the uncertainty contribution of this realization. [4.3].

#### 4.1 *The role and status of the international prototype*

The mass values of the IPK and its six official copies are now determined experimentally by traceability to primary mass standards (see Section 3).

Subsequent changes to the mass of the IPK may have historical interest even though the IPK no longer retains a special status or a dedicated role in the *mise en pratique* [4.4]. By following the change in mass of the IPK over time, one may be able to ascertain its mass stability with respect to fundamental constants, which has long been a topic of conjecture. For that reason, the IPK and its six official copies are conserved at the BIPM under the same conditions as they were prior to the redefinition.

## 5. References

(*Editor's note 5.1*: A special issue of Metrologia will be published that will contain explanations of this *mise en pratique*. Then, at least the references 2.2, 2.3, 2.4, 2.5, 3.5, 4.3, and 4.4 can refer to the special issue.)

- [1.1] *SI Brochure* published following adoption of the “New SI” (9th edition)
- [1.2] Last CODATA Least Squares Adjustment of the fundamental constants, prior to the adoption of the “New SI” by the CGPM.
  
- [2.1] [OIML D28 \(2004\)](#), 12 pp. See Note 1 on p. 3
- [2.2] Selection of available review article(s) on watt balances
- [2.3] Review article on electromagnetic and electrostatic techniques other than watt balances, e. g. “Recent Development on Joule Balance at NIM,” IEEE Trans. Instrum. Meas., Vol. 60, No. 7, pp. 2533-8 (2011)
- [2.4] CODATA chapter on  $h/m(X)$  or review article
- [2.5] Best available review article(s) on XRCD
  
- [3.1] *Measurement comparisons in the CIPM MRA*, CIPM MRA-D-05, Version 1.2, [http://www.bipm.org/utis/common/CIPM\\_MRA/CIPM\\_MRA-D-05.pdf](http://www.bipm.org/utis/common/CIPM_MRA/CIPM_MRA-D-05.pdf)
- [3.2] Link to BIPM.M-K1
- [3.3] *Traceability in the CIPM MRA*, CIPM 2009-24 (revised 13 October 2009) [http://www.bipm.org/cc/CIPM/Allowed/98/CIPM2009\\_24\\_TRAC\\_MRA\\_RE\\_V\\_13\\_OCT\\_2009.pdf](http://www.bipm.org/cc/CIPM/Allowed/98/CIPM2009_24_TRAC_MRA_RE_V_13_OCT_2009.pdf)

- [3.4] Resolution 1 of 24th CGPM (2011) and Resolution 1 of the 25th CGPM (2014)
- [3.5] Paper on the BIPM ensemble of reference mass standards
  
- [4.1] Publication of the “Extraordinary Calibrations using the IPK”.
- [4.2] Publication of the pilot study.
- [4.3] Paper on transition from old to new definition.
- [4.4] Davis, R.S. “The role of the international prototype of the kilogram after redefinition of the International System of Units”, *Phil. Trans. R. Soc. A*, 2011, **369** 3975-3992, or something similar.
  
- [A2.1] *Mise en pratique* of the (new) kelvin.
- [A2.2] CODATA LSA after redefinition.



# ANNEXES

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(*Editor's note A0.1*: A special issue of Metrologia will be published that will contain explanations of this *mise en pratique*. Then, most part of the annexes can be replaced by references to this special issue.)

## A1. History leading to the redefinition of the kilogram

In 1993, following publication of the results of the Third Verification of national prototypes of the kilogram (1988-1992), the CCM and the CIPM formally recommended that experiments be pursued in order to monitor the stability of the international prototype of the kilogram by “independent methods”. This opened the way for a redefinition of the kilogram in terms of fundamental constants. Subsequently, identical wording was adopted in Resolution 5 of the 20<sup>th</sup> CGPM (1995).

In 1999, the 21<sup>st</sup> CGPM recommended in its Resolution 7 that national laboratories continue their efforts to refine experiments that link the unit of mass to fundamental or atomic constants with a view to a future redefinition of the kilogram.

In 2005 the CCM recommended (CCM Recommendation G1, 2005) that certain conditions be met before the kilogram is redefined with respect to a fundamental or atomic constant. Amongst these were that a *mise en pratique* for the realization of the new definition of the kilogram be drawn up that includes recommendations concerning the various linking experiments, as well as a recommendation for the continuing use of the present artefact, the IPK, to maintain the present excellent worldwide uniformity of mass standards.<sup>6</sup> The same year, the CIPM recommended (CIPM Recommendation 1, CI-2005) that, in preparation for redefinitions of several of the SI base units, National Metrology Institutes

- should pursue vigorously their work presently underway aimed at providing the best possible values of the fundamental constants needed for the redefinitions now being considered;
- should prepare for the long term maintenance of those experiments that will, in due course, be necessary for the practical realization (*mise en pratique*) of the new definitions.

The 23<sup>rd</sup> CGPM (2007) recommended in its Resolution 12 that National Metrology Institutes and the BIPM

- pursue the relevant experiments so that the International Committee [for Weights and Measures, CIPM] can come to a view on whether it may be possible to redefine the kilogram, the ampere, the kelvin, and the mole using

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<sup>6</sup> After redefinition, the IPK became a secondary standard as described in Section 4.

fixed values of the fundamental constants at the time of the 24<sup>th</sup> General Conference (2011),

- should, together with the International Committee, its Consultative Committees, and appropriate working groups, work on practical ways of realizing any new definitions based on fixed values of the fundamental constants, prepare a *mise en pratique* for each of them, and consider the most appropriate way of explaining the new definitions to users,
- initiate awareness campaigns to alert user communities to the possibility of redefinitions and that the technical and legislative implications of such redefinitions and their practical realizations be carefully discussed and considered,

and requested that the CIPM report on these issues to the 24<sup>th</sup> CGPM in 2011 and undertake whatever preparations are considered necessary so that, if the results of experiments were found to be satisfactory and the needs of users met, formal proposals for changes in the definitions of the kilogram, ampere, the kelvin and mole could be put to the 24<sup>th</sup> General Conference.

In 2010, CCM recommendation G1 (2010) reaffirmed the conditions to be met before the kilogram is redefined with respect to a fundamental constant.

Resolution 1 of the 24<sup>th</sup> CGPM (2011) noted the intention of the International Committee for Weights and Measures (CIPM) to propose a revision of the SI. It further encouraged

- researchers in national metrology institutes, the BIPM and academic institutions to continue their efforts and make known to the scientific community in general and to CODATA [specifically, to the Task Group on Fundamental Constants (TGFC) of the Committee on Data of the Committee for Data in Science and Technology (CODATA)] in particular, the outcome of their work relevant to the determination of the constants  $h$ ,  $e$ ,  $k$ , and  $N_A$ , and
- the BIPM to continue its work on relating the traceability of the prototypes it maintains to the IPK, and in developing a pool of reference standards to facilitate the dissemination of the unit of mass when redefined,

and invited the CIPM to make a proposal for the revision of the SI as soon as the recommendations of Resolution 12 of the 23<sup>rd</sup> meeting of the General Conference are fulfilled, in particular the preparation of *mises en pratique* for the new definitions of the kilogram, ampere, kelvin and mole.

In 2013 the CCM confirmed and clarified in its Recommendation G1 (2013) the conditions to be met before the kilogram is redefined with respect to a fundamental constant.

Resolution 1 of the 25<sup>th</sup> CGPM (2014) confirmed the intention to carry out the plan of Resolution 1 of the 24<sup>th</sup> CGPM (2011) as soon as the conditions laid out in Resolution 1 are met and presumed this would be possible by the time of the 26<sup>th</sup> meeting of the CGPM in 2018.

## A2. Traceability to units derived from the kilogram

### A2.1. Coherent derived units expressed in terms of base units $kg\ m^p\ s^q$

Neither the realizations of the metre nor the second have been affected by the Resolution XX of the XXth CGPM. This means that for any coherent derived units expressed in terms of base units as  $kg\ m^p\ s^q$  (where  $p$  and  $q$  are integers), the only change in traceability to the SI is in the traceability to the kilogram, and this has been described above. Examples of quantities and their associated coherent derived units are shown in Table A2.1. Several of the coherent derived units have special names, e.g. newton, joule, pascal. These are not given in Table A2.1 but they are tabulated in Table 5 of the 9th edition of the *SI Brochure* [1.1].

Table A2.1. Some quantities whose SI coherent unit is expressed as  $kg\ m^p\ s^q$ .

quantity	p	q
mass density	-3	0
surface density	-2	0
pressure, stress	-1	-2
momentum	1	-1
force	1	-2
angular momentum	2	-1
energy, work, torque	2	-2
power	2	-3

### A2.2. Electrical units

The ampere was previously defined in terms of the second, the metre and the kilogram, and by giving a fixed numerical value to the magnetic constant  $\mu_0$ , whose unit is  $kg\ m\ s^{-2}\ A^{-2}$  (equivalently,  $N\ A^{-2}$  or  $H\ m^{-1}$ ). The ampere is now defined in terms of the second and a fixed numerical value for the elementary charge  $e$ , whose unit is  $A\ s$ . The fact that the Planck constant now has a defined numerical value is of great utility to electrical metrology, as described in the *mise en pratique* for the ampere.

### A2.3. Units involving the kelvin and the candela

The kelvin is now defined in terms of the second, the metre, the kilogram and an exact value for the Boltzmann constant  $k$ , whose unit is  $kg\ m^2\ s^{-2}\ K^{-1}$  (equivalently,  $J\ K^{-1}$ ). The redefinition of the kilogram has no practical impact on this change (see the *mise en pratique* of the definition of the kelvin [A2.1]). Similarly, although the definition of the candela refers in part to an energy, Resolution XX has had no practical impact on the realization of the candela.

### A2.4. Atomic, subatomic and molecular units

(Note: This section focuses on atomic physics rather than chemistry.)

The fact that adoption of Resolution XX by the XXth CGPM (20XX) redefined both the kilogram and the mole, and that the unit of molar mass is  $kg\ mol^{-1}$ , is a potential source of confusion regarding non-SI units such as the unified atomic mass unit,  $u$ , commonly used in atomic, subatomic and molecular science. The following describes

the present situation and contrasts it with the situation prior to the adoption of Resolution **XX**. In Section A2.4.1 we list important equations used in atomic and molecular physics and define the quantities that appear in these equations. Of course the changes to the SI have no effect on the equations. However, uncertainties of the quantities appearing in the equations are affected by the redefinitions of the kilogram and mole. Section A2.4.2 describes these changes and gives present uncertainties.

#### A2.4.1. What has not changed

The equations of physics have not changed. Some of the principal relations used in atomic physics are recalled in this subsection.

The unified atomic mass constant  $m_u$  is defined in terms of the mass of the  $^{12}\text{C}$  isotope

$$m_u = m(^{12}\text{C})/12 . \quad (\text{A2.1})$$

The unified atomic mass unit,  $u$ , also known as the dalton (symbol: Da), is not an SI unit. Formally, the conversion between  $u$  and kg is  $u = \{m_u\} \text{ kg}$  where the curly brackets around  $m_u$  mean “the numerical value of  $m_u$  when it is expressed in the unit kg”.

The relative atomic mass of an elementary entity  $X$  is defined by

$$A_r(X) = m(X)/m_u = 12m(X)/m(^{12}\text{C}) \quad (\text{A2.2})$$

where  $A_r(X)$  is the relative atomic mass of  $X$ , and  $m(X)$  is the mass of  $X$ . (Relative atomic mass is usually called “atomic weight” in the field of chemistry.) The elementary entity  $X$  must be specified in each case. If  $X$  represents an atomic species, or nuclide, then the notation  $^A X$  is used for a neutral atom where  $A$  is the number of nucleons; for example:  $^{12}\text{C}$ .

In the SI,  $m_u$  is determined experimentally in terms of the definition of the kilogram. See the next section for additional information.

The molar mass of  $X$ ,  $M(X)$ , is defined as the mass of the entity  $X$  multiplied by the Avogadro constant,  $N_A$ . The SI coherent unit of  $M(X)$  is  $\text{kg mol}^{-1}$ . For any elementary entity  $X$ ,  $M(X)$  is related to  $m(X)$  through  $N_A$ :

$$M(X) = m(X)N_A = A_r(X)m_u N_A. \quad (\text{A2.3})$$

The molar mass constant  $M_u$  is defined as

$$M_u = M(^{12}\text{C})/12 . \quad (\text{A2.4})$$

These four equations relate the various quantities which are the building blocks of atomic and molar masses and, by extension, are often applied to subatomic and molecular masses.

#### A2.4.2 What has changed

To discuss the changes to the SI, we begin with two additional equations taken from the Rydberg relation of atomic physics,

$$hR_\infty = \frac{1}{2} m_e \alpha^2 c, \quad (\text{A2.5})$$

where  $R_\infty$  is the Rydberg constant,  $m_e \equiv m(\text{e})$  is the electron rest mass,  $\alpha$  is the fine structure constant and  $c$  is the speed of light in vacuum.

First, it follows from (A2.2) and (A2.5) that for any entity X,

$$\frac{h}{m(\text{X})} = \frac{1}{2} \frac{A_r(\text{e})}{A_r(\text{X})} \frac{\alpha^2 c}{R_\infty}. \quad (\text{A2.6})$$

Second, from (A2.3), (A2.4) and (A2.6),

$$\frac{N_A h}{M_u} = \frac{1}{2} A_r(\text{e}) \frac{\alpha^2 c}{R_\infty}. \quad (\text{A2.7})$$

The right-hand side of (A2.7), which is traceable to the SI units of time and length, has a relative standard uncertainty of  $\text{X.X} \times 10^{-10}$  [A2.2]. This relation is key to understanding how the uncertainties of  $M_u$  and  $m_u$  were affected by Resolution XX of the XXth CGPM (20XX).

Of the constants appearing in the eight relations shown above,  $M_u$  (and by extension  $M(^{12}\text{C})$ ), had a fixed numerical value before the SI was reformulated by the XXth CGPM, but no longer. The constants  $N_A$  and  $h$  did not have fixed numerical values previous to the XXth CGPM. (The numerical value of the speed of light in vacuum, whose SI coherent unit is  $\text{m s}^{-1}$ , has been specified exactly since 1986).

Thus Resolution XX of the XXth CGPM has had the following consequences to the quantities and measurements discussed above:

1. Relative atomic masses (usually referred to as atomic weights in the field of chemistry) are unaffected. They are dimensionless ratios and thus independent of unit systems.
2. Experiments to determine the fine structure constant are unaffected.
- 3a. Neither the value nor the uncertainty of  $N_A h/M_u$  were affected by Resolution XX. The value of this combination of constants is still determined from the recommended values for the parameters on the right-hand side of (A2.7), and these are either traceable to SI units of time and length, or are dimensionless [A2.2].

In some scientific papers published prior to the adoption of Resolution XX, the quantity  $N_A h/M_u$  has been written as  $N_A h(10^3)$ , where the factor  $10^3$  was used as a kind of short-hand to indicate the exact numerical value of  $M_u^{-1}$  whose SI coherent unit is  $\text{mol kg}^{-1}$ . This short-hand was acceptable when the mole was defined through the definition of the kilogram combined with an exact numerical value of  $M_u$ ; but the mole is now defined through a fixed numerical value of  $N_A$ , whose SI coherent unit is

$\text{mol}^{-1}$ . Nevertheless,  $M_{\text{u}}$  may still be taken to be exactly  $0.001 \text{ kg mol}^{-1}$  as long as the relative standard uncertainty of  $M_{\text{u}}$ , which is currently  $\text{X.X} \times 10^{-10}$  [A2.2], can be neglected—both conceptually and in the uncertainty budget of a measurement under discussion.

3b. For no other reason than to bring clarity to the discussion in this subsection, the changes to the value of  $M_{\text{u}}$  and its uncertainty may be parameterized in terms of a small, dimensionless quantity  $\kappa$ . The molar mass constant  $M_{\text{u}}$ , instead of being defined as exactly  $0.001 \text{ kg mol}^{-1}$ , as it was prior to the adoption of Resolution **XX**, can be accurately derived from the last term of the following relation

$$M_{\text{u}} = (0.001 \text{ kg mol}^{-1})(1 + \kappa) = \frac{R_{\infty}}{A_{\text{r}}(\text{e})\alpha^2} \left( \frac{2N_{\text{A}}h}{c} \right), \quad (\text{A2.8})$$

where, in the last term, the constants in the final parentheses have exactly defined values.

Due to the principle of continuity when changes are made to the SI, the value of  $\kappa$  is consistent with zero to a relative standard uncertainty of  $u_{\text{r}}(\kappa) = u_{\text{r}}(R_{\infty}/(A_{\text{r}}(\text{e})\alpha^2))$ , which at present is  $\text{X.X}$  parts in  $10^{10}$ . This uncertainty would be further reduced by improved measurements of the constants involved,  $\alpha$  in particular. The accepted values and relative uncertainties of  $A_{\text{r}}(\text{e})$ ,  $R_{\infty}$  and  $\alpha$  are the CODATA recommended values [A2.2], found on-line at:

<http://physics.nist.gov/cuu/Constants/index.html>.

The molar mass constant and the unified atomic mass constant are related by  $M_{\text{u}} = m_{\text{u}}N_{\text{A}}$ . It follows that, since  $u_{\text{r}}(N_{\text{A}}) = 0$ , the relative uncertainties of  $m_{\text{u}}$  and  $M_{\text{u}}$  are identical:

$$u_{\text{r}}(m_{\text{u}}) = u_{\text{r}}(M_{\text{u}}) = u_{\text{r}}(\kappa). \quad (\text{A2.9})$$

For the case of  $m_{\text{u}}$ , whose value has been (and remains) determined by experiment, the adoption of Resolution **XX** nevertheless resulted in a reduction of  $u_{\text{r}}(m_{\text{u}})$  by nearly a factor of **70 [ToBeConfirmed]** simply by defining  $h$  to have a fixed numerical value, although this improved uncertainty does not seem to have any immediate practical benefits.

### A3. Maintenance of primary realizations

In the past, an experiment capable of determining the value of the Planck constant provided a result of enduring value, even if the experiment was never repeated. Now that similar experiments are used to realize the mass unit, we discuss briefly whether an abbreviated experiment could be used to ensure that the realization remains valid. If we consider the realizations described in Section 2, the basic question is: must routine realizations of primary mass standards be identical to the first such realization? Some considerations are given here.

For realization through a watt balance: Assurances are needed that the mechanical and magnetic alignments of the balance remain adequate; that SI traceability is maintained to auxiliary measurements of velocity, gravitational acceleration, current and voltage.

Improved technology in these areas opens the possibility of reducing the uncertainty of the realization.

For a realization through XRCD,  $^{28}\text{Si}$ -enriched, single-crystal silicon was prepared under the auspices of the International Avogadro Coordination (IAC). X-ray interferometers, samples for molar mass measurements, two 1 kg spheres for the density measurement, and many other samples were prepared from the same ingot. The spheres are primary mass standards from which the mass unit can be disseminated, but the spheres must be maintained in good condition for periodic monitoring by appropriate methods of the following parameters:

- Surface layers on the silicon spheres by, for example, spectral ellipsometry, X-ray refractometry (XRR), X-ray photoelectron spectrometry (XPS), X-ray fluorescence (XRF) analysis, and infrared absorption;
- Volume of the silicon spheres by, for example, optical interferometry.

These measurements are not onerous and it is estimated that they could be carried out within a few weeks.

In addition, although no known mechanism would change the molar mass of the crystals, re-measurement of the molar mass by improved methods could reduce the uncertainty with which the kilogram definition can be realized by the XRCD method.

Similarly, there is no known mechanism for the edge dimension  $a(\text{Si})$  of the unit cell to change with respect to time, but re-measurement of this quantity by combined X-ray and optical interferometry could reduce the uncertainty with which the kilogram definition can be realized by the XRCD method.

Confirmation can be provided by mechanisms of the CIPM MRA, which provide measures of the equivalence of the various realizations.

#### **A4. Maintenance of mass correlation among artefacts calibrated by NMIs or DIs realizing the kilogram (optional)**

In the context of the CIPM MRA, an NMI, DI or the BIPM, realizing the mass unit would be able to calibrate mass standards traceable to their own realization only, provided that the laboratory has participated with success in a key comparison as described in section 3.1. However, as long as the uncertainty of a primary realization is significantly larger than the uncertainty of a mass comparison, the uncertainty of a calibration traceable to a single realization would be larger than the uncertainty of a calibration traceable to multiple realizations at least in the case of independent and consistent results.

Laboratories realizing the mass unit might take advantage of the information obtained in key comparisons in order to reduce the mass calibration uncertainty and increase the correlation of mass measurement worldwide. The following simplified example illustrates how the analysis of the key comparison might be modified in order to achieve this.

Assume that a number  $n$  of laboratories is realizing the mass unit. These laboratories are labeled  $\text{NMI}_1, \dots, \text{NMI}_n$ . As a result of the realization,  $\text{NMI}_i$  assigns a prior value  $m_i$  and an associated standard uncertainty  $u(m_i)$  to a stable mass standard  $S_i$  with nominal mass 1 kg. In a subsequent key comparison,  $\text{NMI}_i$  measures the mass difference between the standard  $S_i$  and a circulated, stable mass standard  $S_R$ .  $\text{NMI}_i$  reports the measured mass difference  $\Delta m_i$ , the prior mass value  $m_i$  and the associated standard uncertainties  $u(\Delta m_i)$  and  $u(m_i)$ .

The key comparison reference value  $\hat{m}_R$  (the mass of the circulated standard  $S_R$ ) and highly correlated posterior values  $\hat{m}_i$  of the mass standards  $S_i$  are obtained as the weighted least squares solution to the model

$$\begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ m_n \\ \Delta m_1 \\ \Delta m_2 \\ \vdots \\ \Delta m_n \end{pmatrix} \square \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 1 & 0 & \cdots & 0 & -1 \\ 0 & 1 & \cdots & 0 & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -1 \end{pmatrix} \begin{pmatrix} \hat{m}_1 \\ \hat{m}_2 \\ \vdots \\ \hat{m}_n \\ \hat{m}_R \end{pmatrix}$$

(The symbol  $\square$ , also used in [1.2], indicates that an input datum of the type on the left-hand side is ideally given by the expression on the right-hand side containing adjusted quantities.)

In the subsequent dissemination of mass unit,  $\text{NMI}_i$  uses the stable mass standard  $S_i$  as reference, but with the posterior value  $\hat{m}_i$  and associated standard uncertainty  $u(\hat{m}_i)$  rather than the prior value  $m_i$  and associated standard uncertainty  $u(m_i)$ .

For simplicity, the above example is based on the assumption that stable mass standards are available. Such standards were not available in the past, and they may not be available in the future either. However, as long as the changes in mass standards are predictable with an uncertainty smaller than the uncertainty of the realization of the mass unit, a procedure similar to the one described, but which takes into account the instability of the mass standards, will provide posterior mass values with smaller uncertainties and higher correlations than those of the prior values.



## History of the document:

Version	Date	Authors	Remarks
1.0	10.06.2010	Davis & Picard	Initial version
1.1	22.07.2010	Richard	Comments of Richard included
1.3	08.08.2010	Richard	Comments of Davis, Picard included
1.4	30.09.2010	Richard	Comments of Jabbour, Bich, Thomas, Fujii, Gläser, Borys, Nielsen included
1.51	17.01.2011	Richard	Version with notes and possible authors for the different sections in preparation of the 13 <sup>th</sup> CCM (2011).
1.52	19.01.2011	Richard	Modification of the authors according to Picard
2.0	05.02.2011	Davis	Preliminary synthesis document
3.0	23.08.2011	Davis	First Draft of coherent synthesis document. Edited as if the <i>mise en pratique</i> has been written following the redefinition of the kilogram instead of in anticipation of the redefinition.
4.0	12.12.2011	Davis	Based on a meeting with Richard 19.10.2011, the following major changes made: In general, <u>all</u> equations in the text have been numbered. Following sections changed: 1. (last two paragraphs deleted.) 1.2.1 (specified that the major topic of the MeP is realization of the unit at a nominal value of <u>1 kg</u> ) 1.2.2 (moved to Annex 2) 2.3 (becomes 2.1) In the new 2.2, first paragraph is deleted; some information moved to footnotes; place-holders are indicated for key references; next-to-last paragraph deleted. 3. (sent to co-authors for re-write, with final editing to be done by Davis) 4. Last two sentences of second paragraph deleted. 4.2. Moved to Annex.
5.0	18.03.2012	Davis	Removal of authors' names from individual sections. Text in Section 3 has been added or revised following submission or resubmission by the authors.
5.1	19.03.2012	Davis	Elimination of several annexes now considered to be unnecessary.

5.2	20.04.2012	Richard	Minor editorial revision and simplification. This version was circulated to WGSi-kg for comment.
6.0	30.09.2012	Davis	Comments from members of WGSi-kg incorporated as follows: 1. Suggestions implemented to correct errors, to improve formatting or to add what is considered by some to be essential details. 2. Issues that remain contentious clearly require further discussion and the Workshop is the place for this. Editor's notes are included in red to highlight the most fundamental disagreements among comments received from the WGSi-kg. Resolution of these points is required. 3. Annex A4 which was not included in version 5.2 has not yet been commented on by the WGSi-kg. This Annex is related to one of the contentious issues highlighted in the text.
6.1;6.2;6.3	02.10.2012	Davis & Richard	Minor editorial changes
7.0	02.04.2013	Davis	Following comments on v.6.3
7.1	27.02.2013	Davis	Editorial changes shown in blue made following meeting of CCM WGSi-kg
8.0	13.06.2013	Bettin & Davis & Milton & Richard	Following comments and suggestions received on draft 7.1.
8.1	16.08.2013		
8.2	27.08.2013		
8.3	02.09.2013		
8.4	13.11.2013		
8.5	17.11.2013		
8.6	27.11.2013		
8.7	12.12.2013		
9.0	10.12.2014	Bettin&Davis	Following comments and suggestions received on draft 8.7 and actions of the 25th meeting of the CGPM (2014)