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A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities

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A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities

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Prologue

In the proposed new SI, the kilogram will be redefined in terms of the Planck constant and the mole will be redefined in terms of the Avogadro constant. These redefinitions will have some consequences for measurements in chemistry. The goal of the Mole Project (IUPAC Project Number 2013-048-1-100) was to compile published work related to the definition of the quantity ‘amount of substance’, its unit the ‘mole’, and the consequence of these definitions on the unit of the quantity mass, the kilogram. The published work has been reviewed critically with the aim of assembling all possible aspects in order to enable IUPAC to judge the adequateness of the existing definitions or new proposals. Compilation and critical review relies on the broadest spectrum of interested IUPAC members.

1 Introduction

> ”It is as easy to count atomies as to resolve the propositions of a lover.”
> William Shakespeare, *As You Like It*

The International System of Units (SI) is defined and published in the SI Brochure produced by the International Committee for Weights and Measures (CIPM) at the request of the General Conference on Weights and Measures (CGPM). The Brochure is currently in its 8th Edition since 1970. The main purpose of this document is ”to define and promote the SI, which has been used around the world as the preferred language of science and technology since its adoption in 1960 through a Resolution of the 11th General Conference on Weights and Measures” [1].

Table 1: Comparison between the current SI [1] and the proposed new SI [2] for the definitions of the kilogram and the mole. This 2011 text of the proposed new SI is not necessarily the final wording that will be recommended by the CIPM to the CGPM prior to the next CGPM meeting in 2018. The numbers given in the last column (proposed new SI) have been modified according to the CODATA 2014 recommendation [3]. Final values will be computed by CODATA prior to introduction of the new SI.

Base Quantity, Unit Name	*Current SI* [1]	*Proposed new SI* [2]
mass, the kilogram	The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram.	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 $6.626\,070\,040 \times 10^{-34}$ when it is expressed in the SI unit for action J s = kg m^2 s^{-1}.
amount of substance, the mole	1. The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12; its symbol is ”mol”. 2. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.	The mole, symbol mol, is the SI unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles; its magnitude is set by fixing the numerical value of the Avogadro constant to be exactly $6.022\,140\,857 \times 10^{23}$ when it is expressed in the SI unit mol^{-1}.

Resolutions and Recommendations of the CGPM and the CIPM related to the SI are listed in the SI Brochure [1].

Among its principal goals, the proposed new SI is intended to redefine the kilogram. The international prototype kilogram (IPK) is an artifact stored at the BIPM near Paris since 1889. The mass m_{IPK} of the IPK is 1 kg by definition; the artifact is a platinum-iridium cylinder with a height and diameter of approximately 39 mm. Six additional official copies exist. The mass of the IPK and of prototypes in national laboratories have been compared about every 40 years. It turned out that the prototype kilogram and the six official copies showed some divergence in mass over time and relative changes are observed on the order of 5×10^{-8} per century with respect to their first calibration, although this trend was not observed between the two most recent measurement campaigns [4].

The proposed new SI will redefine the kilogram in terms of physical constants. It is planned to redefine the kilogram by fixing the numerical value of Planck constant h. Table 1 compares the current and the future definitions for the SI units kilogram and mole proposed in 2011 [2]. The base unit kilogram influences three other base units in the current SI, namely the ampere, the mole and the candela. At the same time when the kilogram is redefined, it is also intended to redefine three other base units: the ampere, the kelvin and the mole. The new definition of the kilogram by fixing the numerical value of the Planck constant and the new definiton of the mole by fixing the the numerical value of the Avogadro constant N_{A} have implications for chemistry and provoked criticism. Whether or not those implications are of any practical importance will be analysed in the present work.

The quantities m_{u} (atomic mass constant), M_{u} (molar mass constant), A_{r} (relative atomic mass or "atomic weight"), m_{a} (atomic mass), M (molar mass), and N_{A} (Avogadro constant) are particularly important in chemistry, as chemists often determine amount of substance by weighing. These quantities are related for one particular entity X as follows:

$$M(\mathrm{X}) = A_{\mathrm{r}}(\mathrm{X})\ M_{\mathrm{u}} \tag{1}$$

$$M(\mathrm{X}) = N_{\mathrm{A}}\ m_{\mathrm{a}}(\mathrm{X}) \tag{2}$$

$$m_{\mathrm{a}}(\mathrm{X}) = A_{\mathrm{r}}(\mathrm{X})\ m_{\mathrm{u}} \tag{3}$$

Combining Eqs. (1) to (3) results in

$$M_{\mathrm{u}} = N_{\mathrm{A}}\ m_{\mathrm{u}} \tag{4}$$

The amount of substance X, $n(\mathrm{X})$, is given as

$$n(\mathrm{X}) = N(\mathrm{X})/N_\mathrm{A} \tag{5}$$

where $N(\mathrm{X})$ denotes the number of entities X. Eqs. (2), (4) and (5) are of special importance for chemistry because they connect the mass of an individual entity (microscopic mass) with the mass (usually macroscopic) of an arbitrary number of the same entities, similar to

$$F = N_\mathrm{A}\; e \tag{6}$$

and

$$R = N_\mathrm{A}\; k \tag{7}$$

which connect the Faraday constant F to the elementary charge e, and the Boltzmann constant k to the universal gas constant R. The Avogadro constant and the Planck constant are related by

$$\frac{\alpha^2\, A_\mathrm{r}(\mathrm{e})\, M_\mathrm{u}\, c_0}{2\, R_\infty} = N_\mathrm{A}\; h \tag{8}$$

to the Rydberg constant R_∞, the fine-structure constant α, the relative atomic mass of the electron $A_\mathrm{r}(\mathrm{e})$, the speed of light in vacuum c_0 and the molar mass constant M_u.

In order to prepare a critical assessment of facts and opinons about the two changes in the SI that are most important for chemists, the new definition of the kilogram and that of the mole, three IUPAC divisions, Divisions I, II and V, the Committee for Chemical Education (CCE) and the Interdivisional Committee for Terminology, Nomenclature and Symbols (ICTNS), have jointly launched a project in 2013, the outcome of which is the present Technical Report. An initial meeting was held in Paris by J. Meija, Z. Mester, and J. Stohner in April 2014. In July 2014, the first meeting involving all task group members was held in Zurich to distribute tasks and to start reviewing relevant literature. The second meeting, where this Technical Report was started, was held in Ottawa end of January 2015. The minutes of all meetings are published on the IUPAC website [5,6] and attached to this paper as an electronic supplementary information.

The outline of this document is as follows. After the introduction, Section 2 summarizes briefly the history of the determination of the Avogadro constant and the evolution of its numerical value over time. A short paragraph is devoted to the history of the process by which the positioning within IUPAC in reference to the proposed new SI was reached before this task group was created. Section 3 describes the new SI and its special relation to the chemistry community. Section 4 briefly describes our strategy to assess the community's attitude towards the new SI, mainly by conducting a written survey among the National Adhering Organizations (NAOs) to IUPAC. Section 5 reviews articles in favor or against the proposed new SI and summarizes their major points. We have covered the published literature which appeared prior to the Ottawa meeting in January 2015 and a few more papers that appeared since then. Section 6 presents the results and feedback from the survey of the NAOs. Section 7 concludes the critical assessment.

Based on its critical work, the Task Group quite naturally developed its own consolidated position with respect to the mole and the name of the quantity 'amount of substance'. This position is formulated in an Epilogue, and might be of help to IUPAC to review the position of the Union with respect to the proposed new SI.

2 History

2.1 The mole - A historical flashback

The amount of substance plays a major role in chemistry. This was recognized by the scientific community in 1971 through the acceptance of the amount of substance (chemical amount), n, as one of the seven base quantities in the SI with its corresponding base unit mole (symbol: mol) which ultimately led to the introduction of a new constant, the Avogadro constant N_A. The base unit mole was introduced to resolve the confusion between g-mol ('g-Molekül', 'g-Atom', 'g-equivalent', 'g-formula', etc.), which has been used by chemists to refer to a mass equivalent unit, and g, which is a mass unit [7–10], and to introduce quantity calculus into chemistry [11–18] (see also [19] and refs. [12,13] cited therein). We henceforth also carefully distinguish between the physical quantity amount of substance, and the mole as its unit in the SI. Too often, however, this distinction is not made in practice and 'mole' is used to replace 'amount of substance', which is inappropriate.

Two concepts exist in relation to amount of subtance. A 'number of entities' concept can be understood by considering an ideal gas as a limiting case to real gases. It follows from the state equation

$$p\,V = n\,R\,T = n(\mathrm{E})\,k\,N_\mathrm{A}\,T = N(\mathrm{E})\,k\,T \tag{9}$$

that the amount of any ideal gaseous entity E is the same under identical conditions of pressure p, volume V, and thermodynamic temperature T. Thus, the amount of substance $n(\mathrm{E})$ and consequently the number of entities $N(\mathrm{E})$ are independent of the precise nature of the entity E. Equation (9) is the essential summary of the laws of Gay-Lussac and von Humboldt that led Avogadro to formulate his hypothesis in 1811 (see ref. [10] cited in [20]), while debates concerning continuum models of matter continued to exist until about 1900 and beyond [20].

Amount of substance is proportional to the number of entities, the proportionality factor is the reciprocal of the Avogadro constant. Whether this constant is of fundamental nature or not has also been subject of debates. Perrin gave the demonstration that the numerical value of the Avogadro constant is finite and regarded this as a fundamental advance in proffering the existence of molecules [21]. In this context, it is interesting to point to a debate within the CIPM over whether the mole should be adopted as a base unit. Most of the arguments, in favor and against the adoption of the mole as a base unit, that we read today were already raised in 1970. The position that won the day within the CIPM was that IUPAP and IUPAC had both asked for the mole to become a base unit of the SI and there was no compelling reason to refuse this request [22].

Table 2 collects numerical values of the Avogadro constant over time from experiments in kinetic gas theory, diffusion, crystallography, electrolysis, and black-body radiation. The table is far from being complete and more information can be found in references [7, 20, 23–27].

Table 2: Change of the numerical value of the quantity which is presently known to be the Avogadro constant over time. Many values have been taken from a collection presented in [20, 23].

Name	*Year*	*Numerical value*	*Notes*
J.C. Magnenus	~ 1646	$\approx 2 \times 10^{22}$ $^{(*)}$	diffusion of incense burnt in a church [20, 25]
Loschmidt	~ 1865	5.8×10^{23} $^{(*)}$	mean free path in gases [23]
Röntgen, Rayleigh	~ 1890	$(6 \text{ to } 7) \times 10^{23}$	[20]
Ostwald	~ 1899	6.3×10^{23} $^{(*)}$	[23]
Planck	1900	6.175×10^{23}	black-body radiation [20]
Einstein,	1905/6	6.17×10^{23}	[20]
Smoluchowski	1908	6.0×10^{23}	
	1911	6.56×10^{23}	[23]
Perrin	1909	6.5×10^{23}	[20, 21]
Rutherford	1909	6.16×10^{23}	counting α-particles [23]
Millikan	1917	6.064×10^{23}	Faraday's law [23]
DuNouy	~ 1924	6.003×10^{23}	[23]
Kappler	1931	6.059×10^{23}	[23]
Birge	1941	$6.023\,38 \times 10^{23}$	crystal lattice/XRCD $^{(**)}$ [23]
De Bièvre	2001	$6.022\,133\,9 \times 10^{23}$	[28]
Andreas et al.	2011	$6.022\,140\,78(18) \times 10^{23}$	crystal lattice/XRCD $^{(**)}$ [29]
CODATA	2014	$6.022\,140\,857(74) \times 10^{23}$	recommended [3]

$^{(*)}$ Recalculated, numbers originally given in terms of molecules per cm^3 or per piece of incense. $^{(**)}$ XRCD: *X*-ray crystal density.

The current recommended numerical value for the Avogadro constant is given by CODATA as $6.022\,140\,857 \times 10^{23}\ \mathrm{mol}^{-1}$ with a relative standard uncertainty of 1.2×10^{-8} [3].

A second concept can be tied to the stoichiometric equation, which is also central to chemistry. In 1792, the German chemist Richter elaborated a new alternative of quantitative treatment of matter which he coined 'stoichiometry' meaning 'measure of elements' [30]. Since then, chemists have measured matter not only in terms of volume and mass, but also in terms of the amount of substance.

The stoichiometric equation

$$\mathrm{C_2H_4O} = \mathrm{CH_4} + \mathrm{CO} \tag{10}$$

can be interpreted in two ways: For a chemist working in the laboratory, the equation means that one mole of oxirane ($\mathrm{C_2H_4O}$) decomposes under appropriate conditions to form one mole of methane (CH_4) and one mole of carbon monoxide (CO). Note that here, the quantity 'amount of substance' is not conserved, since one mole of oxirane decomposes into two moles of products, namely one mole of methane and one mole of carbon monoxide. However, masses are always conserved, if one neglects the chemically irrelevant relativistic variation of mass related to the reaction enthalpy.

Another example using the concept of stoichiometry is the electrolytic decomposition of water. 9 g water (H_2O) decomposes into 1 g hydrogen (H_2) and 8 g oxygen (O_2) when approximately 96485 coulomb of electricity has been consumed during the electrolysis, therefore, the relation of the mass of hydrogen, $m(\mathrm{H_2})$, and oxygen, $m(\mathrm{O_2})$, found in this experiment is 1:8. This finding follows from Faraday's second law of electrolysis.

Amount of substance allows a quantitive formulation of the law of multiple proportions due to Dalton and Avogadro: The variation $\Delta n(\mathrm{X})$ of the amount of substance of X in the course of a chemical reaction is related to the variation $\Delta n(\mathrm{Y})$ of the amount of substance of Y in the same chemical reaction by a simple ratio $\Delta n(\mathrm{X})/\Delta n(\mathrm{Y}) = \nu_\mathrm{X}/\nu_\mathrm{Y}$, where ν_X and ν_Y are the stoichiometric coefficients of X and Y, respectively, in the stoichiometric equation of that reaction. This relation follows from the defining equation of the extent of reaction, ξ [11]. The same, simple ratio does not hold for the variations, $\Delta m(\mathrm{X})$ and $\Delta m(\mathrm{Y})$, of the masses of the involved substances. However, every molecule can be attributed a characteristic "chemical mass quantity" which we today call molar mass (see Eq. (2)): $M(\mathrm{X}) = m(\mathrm{X})/n(\mathrm{X})$ and $M(\mathrm{Y}) = m(\mathrm{Y})/n(\mathrm{Y})$; note that, while the symbol $m_\mathrm{a}(\mathrm{X})$ in Eq. (2) refers to the mass of one particular entity X, the symbol $m(\mathrm{X})$ refers here to the mass of the amount $n(\mathrm{X})$ of X. The ratio of the variations of masses is expressed in terms of molar masses and stoichiometric coefficients: $\Delta m(\mathrm{X})/\Delta m(\mathrm{Y}) = \nu_\mathrm{X}/\nu_\mathrm{Y} \times M(\mathrm{X})/M(\mathrm{Y})$. As for the total mass, the molar mass is conserved in a chemical reaction within the accuracy of current measurements of mass: $\sum_\mathrm{X} \nu_\mathrm{X} M(\mathrm{X}) = 0$ (the 'reaction mass' is zero). For this reason we may say that, in Eq. (10), 44.053 g oxirane decomposes to yield 16.043 g methane and 28.010 g carbon monoxide, with conservation of mass, because the stoichiometric coefficients there are $\nu_{\mathrm{C_2H_4O}} = -1$, $\nu_{\mathrm{CH_4}} = \nu_{\mathrm{CO}} = 1$, and because these masses are molar masses or mass equivalents; but if we decomposed 1 g of oxirane, we would not get 0.5 g methane and 0.5 g carbon monoxide, despite the fact that masses would be conserved, because the latter masses are not correct molar masses or mass equivalents. We also note that the molar quantities, such as molar mass and molar volume are intensive. They are independent of the number of specified entities in a sample. This number may be as small as one or may be too large to be counted directly.

Working in the laboratory and doing synthesis or electrolysis, however, there is no need to introduce amount of substance as a new quantity; it is sufficient to know the laws of Avogadro, Dalton and Faraday and the molar mass, as the appropriate mass equivalent, for every atom and molecule. The determination of molar masses for any chemical compound has been made possible by the use of the relative atomic mass scale. Consequently, with the use of relative atomic masses (”atomic weights”), chemists are able to convert mass measurements into a quantity that is proportional to the number of entities. The distinction between the chemical amount (1 mol) and the number of entities (about 6×10^{23}), however, still seems to be unclear and might lead to confusion. In principle, both are referring to the same property of matter – the numerosity.

Finally, the aforementioned example of the oxirane decomposition reaction also allows us to interpret amount of substance within its first conceptual frame, namely in chemical kinetics. Eq. (10) enables us to say that one molecule of oxirane decomposes into one molecule of methane and one molecule of carbon monoxide. This interpretation uses a *microscopic* point of view, namely that one possible reaction channel for the decomposition of oxirane is represented as an unimolecular reaction leading to a rate of reaction which is only proportional to the amount concentration (or number density) of oxirane and interpreting

$$\mathrm{C_2H_4O} \rightarrow \mathrm{CH_4} + \mathrm{CO} \tag{11}$$

as a so-called *elementary reaction*. It is usually not permitted to replace the equal sign in the stoichiometric equation by an arrow when entering the field of chemical kinetics [11]. This reaction has been investigated experimentally to determine the Arrhenius parameters of a first order kinetics (see [31, 32] and refs. therein) where the rate of reaction depends only linearly on the amount concentration of oxirane, as indicated in Eq. (11).

We thus have a *macroscopic* and a *microscopic* (particulate) interpretation of the same stoichiometric equation with very different implications. The introduction of the base quantity amount of substance reflects both views: within the first concept, it reflects the microscopic view, within the second concept it reflects the macroscopic view. As mentioned before, the adoption of the mole as a base unit of the SI was made at the joint request of IUPAC, IUPAP and ISO [1] and was agreed to by the CIPM after intense reflection [22].

2.2 History of IUPAC position concerning the proposed new SI prior to the present work

On 9 July 2009, Prof. Mills (the IUPAC Representative to and President of the CCU – Consultative Committee on Units), sent a letter to IUPAC ICTNS Chair Prof. Lorimer informing him of CCU’s intentions to propose the redefinition of several SI base units including the mole. He stated that ”I would like to hear opinions from members of your committee. I certainly wish ICTNS to be aware of this proposal, and I would really like to come away with some expression of support for the proposal or perhaps of opposition, if that should be the case ... The CCU strongly supports making the change to fix the value of N_A." At the ICTNS meeting during the 45th IUPAC General Assembly in Glasgow, the implementation of the new SI and its consequences were part of the Agenda. Among the attendees were: J. Dymond (Div. I), J. Reedijk (Div. II), A. Rauter (Div. III), R. Jones (Div. IV), B. Hibbert (Div. V), P. Fedotov (Div. VI), M. Nordberg (Div. VII), J. Nyitrai (Div. VIII), R. Weir (ICTNS), R. Marquardt (ICTNS), A. Fajgelj, P. De Bièvre, I. Mills, T. Coplen, A.J. Thor (ISO TC-12), and F. Pavese. Documents had been circulated in advance of the meeting. On 3 August 2009, Prof. Mills presented definitions considered by CCU for the kilogram, ampere, kelvin, and mole to fix the numerical values of h, e, k, and N_A, respectively, and a new constant-explicit format for the formal definitions of the base units of the SI. This presentation was followed by a presentation of Prof. De Bièvre. Prof. Lorimer put forward a motion which was adopted by vote following an extended discussion. This motion adopted the 'ICTNS resolution' concerning the proposal by the CCU to redefine the mole.

The recommendation of the CCU of the BIPM is supported by the IUPAC, with the following suggestions:

1. The greatest effort should be made to change the name of the ISQ base quantity amount of substance at the same time that a new definition of the mole is approved.
2. A note should accompany the new definition to explain that the molar mass of ^{12}C will be an experimental quantity, with a relative measurement uncertainty of about $1.4{\times}10^{-9}$. [1]

On 26 August 2009, these decisions were communicated to the IUPAC Bureau by Prof. Lorimer. IUPAC Secretary General, Prof. Black, presented this resolution to the IUPAC Executive Committee at its 141st meeting on 3 to 4 October 2009 (Chile). A motion was made and seconded that the motion proposed by ICTNS be approved. The motion was approved unanimously by the IUPAC Executive Committee. This motion was communicated to BIPM as the official IUPAC position on that matter. The said resolution of the Executive Committee was ratified by the IUPAC Council during its 46th meeting on 3 to 4 August 2011 (Puerto Rico).

Whereas the first draft motion put forward by ICTNS Chair Prof. Lorimer stated that: "The name preferred by IUPAC for the SI base unit is 'chemical amount'", the final motion adopted by vote states that: "The greatest effort should be made to change the name of the ISQ base quantity 'amount of substance' at the same time that a new definition of the mole is approved", summarized in ref. [33].

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[1] Now this value is about 0.45×10^{-9}.

3 Proposed new SI

Resolution 1 of the 24th meeting of the CGPM (2011) [2] introduces the new SI, which will link the definitions of the kilogram, mole, ampere and kelvin to exact numerical values for the Planck constant h, Avogadro constant N_A, elementary charge e and Boltzmann constant k. Referring to [2], Resolution 1 of the 25th meeting (2014) [34] notes that progress has been made and encourages continued effort to allow the 26th CGPM (2018) to adopt a resolution to replace the current SI with the revised SI. References [2] and [34] will be referred to as the 'CGPM Resolutions' in this report.

The definitions of the metre and the second are already linked to exactly defined numerical values for the speed of light in vacuum c_0 and the clock frequency of the caesium-133 atom. One effect of both CGPM Resolutions will be the creation of a revised SI with new definitions of the kilogram, mole, ampere and kelvin based on invariant quantities [34]. By contrast, since 1889 the kilogram has been defined as equal to the mass of an artifact known as the international prototype of the kilogram (IPK). Unfortunately the mass, m_IPK, of the IPK cannot be assumed to be invariant, with the consequence that the magnitude of the unit of mass, the kilogram, tracks any possible changes to the quantity m_IPK. In addition, the IPK has only been used during four measurement campaigns, the first ending in 1889, the second in 1946, the third in 1991 and the fourth just ended. The self-consistency between the mass of the IPK (always taken to be exactly 1 kg) and similar objects stored with it is roughly 75 µg over this period of 125 years; the constancy of m_IPK with respect to true fundamental constants over this period is unknown. Since 1971 the mole has been defined by assigning the exact value 12 g mol^{-1} to the molar mass of unbound carbon-12 at rest and zero kelvin temperature [1], $M(^{12}\mathrm{C})$, with $M(^{12}\mathrm{C}) = 12$ g mol^{-1} (exactly). Thus the present definition of the mole is linked to the mass of the IPK but m_IPK is not a perfectly stable quantity.

The proposed new SI solves the problem of the IPK by linking the kilogram to a fixed numerical value of the Planck constant, h, whose SI unit is kg m^2 s^{-1} (or simply J s because joule is a special name for kg m^2 s^{-2}) and measurements traceable to the SI metre and second, which are already defined in terms of fixed numerical values assigned to two physical constants. The CGPM further proposes to redefine the mole by giving a fixed numerical value to the Avogadro constant, N_A. The choices advocated by the CGPM are not the only possibilities for eliminating the artifact definition of the kilogram and defining the mole. Here we compare in a systematic way the possible approaches available for the redefinition of the mole in order to make these choices and their consequences transparent.

3.1 Choices within constraints

With regard to the definition of the kilogram and the mole in the new SI, we recognize the following constraints:

1. The kilogram can no longer be defined by the mass of a reference artifact.
2. The number of physical constants with fixed values must not over-constrain the SI; there cannot be two independent constants, or groups of constants, that define the same unit.
3. Existing relations among quantities cannot be affected by redefining the units in which the quantities are measured. One of the quantity relations that must remain true under any choice of unit definitions is (see Eq. (2), with X replaced by ^{12}C and $m(\mathrm{X}) = m_\mathrm{a}(^{12}\mathrm{C})$)

   $$m_\mathrm{a}(^{12}\mathrm{C}) = M(^{12}\mathrm{C})/N_\mathrm{A} \tag{12}$$

   where $m_\mathrm{a}(^{12}\mathrm{C})$ is the mass of a neutral atom of carbon-12. The carbon atom is unbound, at rest, and in its ground state thereby ensuring that there are no relativistic corrections to the mass. Eq. (12) is equivalent to Eq.(4).

   Another quantity relation that must remain true under any choice of unit definitions is that given by Eq. (8), which we rewrite here as

   $$\frac{h}{m_\mathrm{u}} = \frac{N_\mathrm{A}\,h}{M_\mathrm{u}} = \frac{c_0}{2}\,\frac{\alpha^2}{R_\infty}\,A_\mathrm{r}(\mathrm{e}) \tag{13}$$

   Note that we cannot fix the values of both h and m_u, or fix the values of the three quantities N_A, h and M_u. Each of these two choices would assign an exact value to the right-hand side of Eq. (13), which is not a logical constraint on the Rydberg constant. The problem is also revealed by noting that $(m_\mathrm{u}c_0^2/h)$, which is a frequency, would have a fixed numerical value thereby redefining the SI unit of time.

   Nevertheless, the relative uncertainty of the experimentally-determined quantity $\alpha^2\,A_\mathrm{r}(\mathrm{e})/R_\infty$ is important because it tells us the relative uncertainty of, say, m_u if the value of h is fixed; or the relative uncertainty of M_u if both N_A and h have fixed values as in the CGPM Resolutions; or the relative uncertainty of h if m_u, N_A and M_u all have fixed values (see Eq. (2)). Eq. (13) also tells us that the principal contribution to the uncertainty of M_u in the revised SI will be that of α^2, uncertainties of the remaining experimental variables being negligible by comparison. From the latest values of the fundamental constants recommended by CODATA [3], we infer that the relative standard uncertainty of the right-hand side of Eq. (13) is 4.5×10^{-10} in the proposed new SI.

Table 3: This table presents the relative standard uncertainties u_r that result from different ways of defining the SI units of importance to chemistry. The resulting u_r are listed for the four constants h: Planck constant (SI unit: kg m^2 s^{-1}), M_u: molar mass constant (SI unit: kg mol^{-1}), N_A: Avogadro constant (SI unit: mol^{-1}), m_u: atomic mass constant (SI unit: kg). The uncertainty of the mass m_IPK is zero in the present SI and entered as Y to indicate a number that will be specified before the proposed new SI is implemented, but which can be expected to be 12×10^{-9} or smaller.

$u_\mathrm{r}(m_\mathrm{IPK})$	$u_\mathrm{r}(h)$	$u_\mathrm{r}(M_\mathrm{u})$	$u_\mathrm{r}(N_\mathrm{A})$	$u_\mathrm{r}(m_\mathrm{u})$	*Notes*
0	12×10^{-9}	0	12×10^{-9}	12×10^{-9}	1 (present SI)
Y	0	0.45×10^{-9}	0	0.45×10^{-9}	2 (proposed new SI)
Y	0	0	0.45×10^{-9}	0.45×10^{-9}	3 (third choice)
Y	0.45×10^{-9}	0	0	0	4 (fourth choice)

(1) At present, the mass of the IPK defines the kilogram and the molar mass constant is defined to be 0.001 kg mol^{-1} (exactly). The values of other quantities are measured experimentally or inferred from experiments by making use of well-known equations: all have identical uncertainties to the precision shown.

(2) The CGPM has resolved to define the kilogram through a fixed numerical value of h, combined with the present definitions for the second and the metre and to define the mole by giving a fixed value to the numerical value of the Avogadro constant in the SI. Consequently the molar mass constant and the atomic mass constant would have equal relative uncertainties inferred from CODATA 2014 [3], although a last CODATA adjustment will be made a few months before the redefinitions are adopted.

(3) The CGPM could have chosen to redefine the kilogram as in Note 2, leaving the definition of the mole unchanged, i.e. fix h without changing the definition of the mole. This would nevertheless have reduced the uncertainties of the Avogadro and atomic mass constants as shown in the table. This is a viable option, however we now have the opportunity to define the mole in a more direct and universal way, similar to the proposed redefinitions of other units.

(4) For chemical measurements a system that fixes the molar mass constant, the Avogadro constant and the atomic mass constant would be very suitable. Note that fixing the values of any two of these constants defines the third through the quantity relation $M_\mathrm{u} = N_\mathrm{A}\, m_\mathrm{u}$. However, in this case m_u defines the kilogram and the value of the Planck constant acquires a finite uncertainty as other constants shown in Note 2 and Note 3; but this uncertainty is not considered to be negligible by electrical metrologists working at national metrology institutes [35, 36].

Table 3 summarizes the relative standard uncertainties u_r on the five quantities most relevant to chemistry (mass of the artifact international prototype of the kilogram, Planck constant, molar mass constant, Avogadro constant, and atomic mass constant) according to different scenarios (Notes 1 to 4). A zero means that the numerical value of the corresponding quantity is exactly defined, or ”fixed”. Non-zero values for uncertainties are taken from the CODATA 2014 recommendations [3] and are expected to be reduced somewhat in a future CODATA adjustment preceding the launch of the new SI. In particular, the relative standard uncertainty of 12×10^{-9} shown in the top row of Table 3 has met the relative uncertainty of 20×10^{-9} recommended by the community of mass metrologists as prerequisite for the redefinition of the kilogram [37].

We may note that the community of mass metrologists, as represented by the Consultative Committee for Mass and Related Quantities (CCM), will realize the new definition of the kilogram in either of two equivalent ways: (1) through a device whose operation resembles that of an analytical balance (the so-called Kibble Watt balance); (2) through a determination of the number of atoms in a pure, monocrystal of silicon-28 whose mass is nominally 1 kg. The latter technique has an additional component of relative standard uncertainty at present equal to 0.45×10^{-9} [3], the same uncertainty shown in Table 3, but this is considered by the research teams to be negligible compared to the total uncertainty budgets of either of the two ways to realize the new definition of the kilogram (see [38,39], however, the uncertainties given therein refer to older values, now superseded [3]).

A short description on how to define the kilogram based on the fixed numerical value of the Planck constant can be found in the Appendix. We describe briefly the crystal density or atom counting approach as well as the Kibble balance (Watt balance), both are currently exploited to link the Planck constant h to the kilogram.

3.2 Consequences for chemistry of the CGPM Resolutions

Consequences for chemistry of the CGPM Resolutions can be evaluated by recalling the following facts: (a) Relations among quantities (such as Eqs. (1) to (9), (12) and (13)) do not depend on any choice of units. As a corollary, changing the definitions of existing units does not (and cannot) introduce any new constants; (b) Ratios of two quantities of the same kind are independent of unit systems and thus immune to any changes of the unit systems, and (c) the unified atomic mass unit, also called the dalton [11], is independent of the SI and therefore unaffected by any changes to the SI. The value of the dalton in SI units will have an uncertainty an order of magnitude smaller in the proposed new SI than at present.

We now consider the following quantities (Item 1. to Item 8.), important for metrology in chemistry (see IUPAC Green Book [11]), and discuss how they might be affected by the new SI:

1. $A_\mathrm{r}(\mathrm{X})$: relative atomic mass of the element X (for historical reasons called 'atomic weight' of X)
2. $M_\mathrm{r}(\mathrm{X})$: relative molar mass of entity X (for historical reasons called 'molecular weight' of entity X)
3. m_u : atomic mass constant; m_u is equal to the unified atomic mass unit, $m_\mathrm{u} = 1$ u. It is used to report masses of nuclides and its value in the SI unit kg is not exact, see

Table 3 Note 2. This unit is a non-SI unit accepted for use with the SI and defined as one twelfth of the mass of an unbound carbon-12 atom at rest and in its ground state. The name dalton, symbol Da, is used as an alternative name for the unified atomic mass unit [11]

4. M_u : molar mass constant

5. N_A : Avogadro constant

6. $m_\mathrm{a}(\mathrm{X})$: atomic mass of entity X, with

$$m_\mathrm{a}(\mathrm{X}) = A_\mathrm{r}(\mathrm{X})\, m_\mathrm{u} \tag{14}$$

7. $M(\mathrm{B})$: molar mass of entity B (see Eq. (1), with X replaced by B)

8. $n(\mathrm{B})$: amount of substance B (chemical amount), with

$$n(\mathrm{B}) = m(\mathrm{B})/M(\mathrm{B}) \tag{15}$$

   where $m(\mathrm{B})$ is the mass of a sample of entities B determined by analytical weighing. Alternatively, $n(\mathrm{B})$ can be determined from the number $N(\mathrm{B})$ of entities in the sample, according to Eq. (5), when X is replaced by B.

At the top of the list, $A_\mathrm{r}(\mathrm{X})$ and $M_\mathrm{r}(\mathrm{X})$ are relative quantities. Their values and uncertainties are unaffected by the CGPM Resolution (or any other choices in Table 3). Specifically, tabulated values in the 'atomic weights' of the elements produced by IUPAC CIAAW [40] are unaffected by any choice of rows in Table 3.

From the principle of continuity that is followed when redefining SI units, the present values of the quantities will be the same as before but their uncertainties will often be different. From Table 3, we see that the relative uncertainties of N_A and m_u will be much reduced from present estimates; in fact the uncertainty of N_A will be zero in the new SI. Therefore SI atomic masses (in kilogram) will be known to a reduced uncertainty, as can be inferred from Item 6. and Table 3. Specifically, the Atomic Mass Evaluations published at regular intervals by IUPAP, in which masses of the nuclides are reported in the unified atomic mass unit, are unaffected by any choices shown in the rows of Table 3.

However, we also see in Table 3 that following the revision of the SI the molar mass constant M_u will no longer be exactly 1 g mol^{-1}, but will acquire a relative standard uncertainty of less than 1 part in 10^9 as inferred from the CODATA 2014 recommendations of the fundamental constants. To assess the importance of this new uncertainty component, it is useful to look at its effect on the estimate of molar mass (Item 7. above). Since $M(\mathrm{B}) = A_\mathrm{r}(\mathrm{B})\, M_\mathrm{u}$ and $A_\mathrm{r}(\mathrm{B})$ is unaffected by the CGPM Resolutions, all molar masses will acquire an additional uncertainty component of less than 1 part in 10^9.

Typically, the molar mass is used to estimate the chemical amount $n(\mathrm{B})$ of entity B in a macroscopic sample of mass $m(\mathrm{B})$, where $m(\mathrm{B})$ is determined by weighing on an analytical balance: $n(\mathrm{B}) = m(\mathrm{B})/M(\mathrm{B})$ (see Item 8. above). The uncertainty of this calculation is dominated by estimates of chemical purity and the accuracy of the analytical weighing. For most chemicals, variability of isotopic abundances must also be considered for high-accuracy work. An additional relative uncertainty of 1 part in 10^9 can be neglected [41–43]. The experimental uncertainty of M_u in the proposed new SI was discussed following Eq. (13), where it is seen to be small and unlikely to increase.

The 'zero reaction mass' related to molar mass conservation in a chemical reaction would hence have an additional relative uncertainty of 1 part in 10^9. Recalling the reaction of Eq. (10), to detect such an additional uncertainty, exactly 44.053 g of oxirane should be decomposed to yield 16.043 g of methane and 28.010 g of carbon monoxide. Aside from the fact that molar masses from standard atomic weights do not have the necessary precision, the exact measurement of such masses by weighing in a conventional chemical experiment seems to be currently unrealistic.

A more fundamental way to think about a relative uncertainty of order 1 part in 10^9 is to consider that it is at this level of accuracy where the assumption of mass conservation in chemical reactions begins to break down. For example, exactly 12 g of unbound carbon-12 atoms is reduced to

$$12\,\mathrm{g} \times \left(1 - \frac{\Delta_\mathrm{f} H_0^0(\mathrm{C,graphite})}{M(^{12}\mathrm{C})\,c_0^2}\right) \qquad (16)$$

when the same number of atoms have formed a graphite crystal [15]. Here $\Delta_\mathrm{f} H_0^0(\mathrm{C,graphite})$ is the standard enthalpy of formation of graphite at zero kelvin temperature. The molar mass equivalent of the energy is this enthalpy divided by c_0^2. Further division by $M(^{12}\mathrm{C})$ gives the mass equivalent relative to the unbound mass of the carbon atoms, approximately 0.66×10^{-9}. The breakdown of mass conservation in chemical reactions, insignificant for normal stoichiometry, is one reason not to insist that a chemist's preference for line 4 of Table 3 be imposed on the entire community of scientists. While lines 2 and 3 are both logically possible, the definition given in line 3 would still require the clarification appended in 1980 to the present definition of the mole [1,44]. The clarification was needed due to the breakdown of conservation of mass, as illustrated in Eq. (16). The definition of the mole in line 2 is independent of mass.

We conclude that the proposed new SI (line 2 in Table 3) is to be preferred over both the third and fourth choices in Table 3.

4 Methodology

To assess and critically review the proposed definitions of fundamental chemical quantities and their impact on chemical communities, a set of about 100 published articles including whole theses and memoranda was identified and classified in the categories “pro”, “contra”, or “neutral” in reference to the proposed new SI and, in particular, in reference to the proposed new definitions of the mole and the kilogram. In these categories, papers have been further classified in respect to their relation to general science, metrology or education issues. Specifically, we identified the following themes:

1. Educational aspects in relation to the mole
2. The Avogadro constant
3. Compatibility aspects between molar mass and relative atomic mass (‘atomic weight’)
4. The “entity” concept
5. Further alternative definitions of the mole
6. On the circularity of the current definition of the mole
7. Name of the quantity “amount of substance”
8. Metrological aspects

An additional assessment was obtained via the answers obtained from NAO bodies to a questionnaire.

The most fundamental chemical quantity is the amount of substance. Consequently, the major part of articles inspected dealt with this quantity and the concept to which it implicitly refers. Another chemically relevant quantity is mass, as it is related to the traditional, and currently accepted definition of the mole. All articles were carefully read and analyzed with regard to the following questions pertaining the amount of substance:

- Is the quantity of any necessity ?
- What are arguments in favor or against its current definition or name?
- What are arguments in favor or against its proposed new definition?
- Are there alternative new definitions for the quantity or its name?
- What are arguments in favor or against the current definition of its unit and its *mise en pratique* (realization)?

The papers were distributed among members of the Task Group who individually read them and collected answers to the aforementioned questions in a table. The result of this work is summarized in the following Section 5. Results from the questionnaire are summarized and analyzed statistically in Section 6.

5 Review of selected papers and summary of key issues raised by the scientific community

Many of the articles analyzed in this work contained similar approaches and contents. We have focussed on reviewing unique contents and conclusions from selected papers, and this review is reported in the present section, where we first address general points raised by the scientific community about the proposed new SI and the definition of the mole, while later giving separate space to specific themes as outlined in the previous section. Where appropriate, a critical assessment of the discussion is amended.

Early in the process of establishing a new SI with relevance to the chemical community, Mills et al. [45] presented the argument for the redefinition of the kilogram by fixing either h or N_A. These authors also argued that there are significant advantages moving from the current mass definition to a constant based formulation while drawbacks were limited. In a new definition of the kilogram that fixes either h or N_A, the uncertainties of values of many fundamental constants (when expressed in SI units) would be reduced significantly and significant advantage to the measurement of electrical quantities would also be gained (see also [35] and Table 3, p. 12). As the single negative effect, they contended that the mass of the international prototype m_IPK would no longer be known exactly (in kg) but would have to be determined by experiment. Metrological aspects will be covered in Subsection 5.8 below.

In a subsequent paper [46], Mills et al. provide a comprehensive assessment of the situation surrounding the redefinition of the mole, treating it the same way as the kilogram, ampere and kelvin in terms of need and mandate for redefinition. They specifically advocate defining the kilogram by fixing the value of the Planck constant instead of the conceptually simpler route of fixing the Avogadro constant and the atomic mass constant, or the dalton. One reason advanced by these authors is the apparent advantage for precise electrical measurements [35], leaving N_A 'free' to be used for the definition of the mole. A second reason, for these authors, is that from a more fundamental physical point of view h plays a more important role than N_A. This is at variance with the view initially presented in ref. [45]. The redefinition of the mole in relation to fixed N_A (together with h, e, and k) will have the effect that other constants become exact, for example the Faraday constant F, the universal gas constant R, the Stefan Boltzmann constant σ and the molar volume of an ideal gas V_m at standard pressure and specified temperature. All these constants are of major practical importance in chemistry and physics.

Various comments and concerns related to the proposals for the new SI are assembled in a website www.metrologybytes.net [17] for discussion. Details of the proposed revision of the SI have been summarized [47]. The proposed explicit-constant formulations of the definitions is said to provide a simple and unambiguous approach applicable both for base and derived units. Here the rationale for the redefinition of the mole is presented specifically as an approach to ”eliminate the present poor understanding of amount of substance, which is independent of mass, and its unit mole, which is a unit to count the number of entities” [47]. Concerns have been raised over the proliferation of correlation among the base units in the proposed new SI and it was criticized that units are defined in terms of a web of interrelated fundamental constants of nature [48, 49], and the spatio-temporal constancy of such a system could only be tested against other similar systems which would not be possible in the case of the proposed new SI, named a ’Zanzibar system’ in ref. [50]. In ref. [51] potentially serious flaws of the proposed new SI have been listed, ranging from ‘wrong definitions of the mole’, the fact that the redefinition of the kilogram relies on special relativity and quantum mechanics and that the redefinitions of the SI units are inconsistent, circular (see also [52]) or even wrong [51].

In reference to the proliferation of correlation argument, we may expect that correlations will remain approximately the same in number as those in the present SI. But this is really a non-issue. The proposed new SI assigns fixed numerical values to seven constants when each is expressed in its SI unit [34]. The Planck and Avogadro constants are among the seven. Any other quantity of interest can be measured in terms of one or more of these defining constants.

In reference to the consistency argument, one must distinguish the physical quantity from a unit used to measure it [53]. In this context, the ’ultimate test of the consistency of physics is made by the measurement of dimensionless constants’ [54]. However, all base quantities are dimensional and ’it is in our best interest to choose some dimensional fundamental constants as the basis of our SI by fixing their numerical values because to test the consistency of physics precisely we need units which are intrinsically stable and universally accessible’ [54].

If a dimensional physical constant is assigned a fixed numerical value, a commonly expressed concern is about the consequences that might arise, should the fixed value somehow be ‘wrong’. For example, suppose the present value of the Planck constant has some unsuspected, small error with relation to the mass of the international prototype of the kilogram. A consequence might be that a more refined realization of the kilogram after redefinition might manifest itself as a corresponding change in the calibration of the highest-accuracy mass standards. In order to minimize serious consequences from such a hypothetical situation, CCM made its recommendations cited above [37]. A pertinent example that the change in definitions of the mole and kilogram will have no consequences in testing physical laws is provided by an experimental test of Einstein’s mass-energy relation, as discussed in Appendix B of [55].

Every revision to the SI brings advantages to some and disadvantages to others. Criticism extended to the time-frame and it was argued that the redefinition should come into effect only when sufficiently low uncertainties could be achieved for the various constants needed for the redefinitions [48, 49, 56, 57]. One might question what exactly 'sufficiently low' uncertainties are. Can these even be defined in natural philosophy? As mentioned above, it is the intrinsic stability of a system of units that counts. From a practical point of view, values of fundamental constants are determined from a least squares analysis such as 'to discern the best values of fundamental constants based on all available data in order to avoid discontinuities of the size of a unit after its redefinition' [54].

The validity of an 'urgent' revision of the SI is questioned [57], arguing that the fundamental constants h and α might not be constant over time. Furthermore, the numerical treatment applied by CODATA to fix the 'reference' values of the fundamental constants at the time of the revision raised some concerns [48, 49]. Various experiments are now or will become available in the near future with higher accuracy than current ones, for example an optical clock based on Al^+ is more accurate than the Cs-clock [58]; these advances should be taken into account [57]. In contrast, other authors see all technical requirements set by CCU close to being met such that no delay is indicated [59] and the CODATA 2014 recommended values and uncertainties [3] give added support to the latter position. The SI being a practical system, the definition of the second will undoubtedly be updated to accommodate optical clocks when they become true clocks rather than spectacularly precise frequency standards, as they are today.

5.1 Educational papers concerned about the mole

One of the anchoring concepts in physics and chemistry is that "matter consists of atoms that have internal structures that dictate their chemical and physical behavior" [60]. The macroscopic quantities that are used by students and faculty within the practice of chemistry contain so many atoms, molecules, ions or elementary particles that they are counted in bunches. The unit of such a bunch may be called the mole. Currently, the mole is defined as being that amount of substance which contains as many elementary entities as there are atoms in 0.012 kg of carbon-12 [61]. The number of entities in one mole of substance is related to the Avogadro constant that is in essence a scaling factor between macroscopic and microscopic, particulate quantities [60, 62, 63].

Evidence from peer-reviewed research on teacher and student understanding of the mole concept strongly suggests that the current definition is not well understood nor is it well communicated in textbooks [62, 64–77]. The classroom contexts of the research with students and teachers span the globe. Studies from Lybeck's lab in Sweden of 30 upper secondary school students and 28 teachers of chemistry indicate that few students and only about three out of 28 teachers use the correct SI definition of the mole [67, 68, 78]. The majority of students and teachers use the notion that one mole equals 'Avogadro number' of entities, like one dozen equals the number 12. One should note that, despite the fact the we all seem to understand what is meant by 'Avogadro number', namely the numerical value of the Avogadro constant (symbol: $\{N_\mathrm{A}\}$), the 'Avogadro number' is not defined in the SI Brochure [1]. The definition of the 'Avogadro number' is implicit in Eq. (5) which, indeed, is an equation cited in [1].

The outcome space developed from Lybeck's interviews indicates that students and teachers are well versed in the quantity calculus needed to move back and forth between the macroscopic and microscopic world. Given that the learning outcome emphasized is the ability to solve quantitative problems, then it is not surprising that the relationship one mole equals 6.022×10^{23} entities serves as a proxy for the definition of the mole (see, for instance ref. [79]). In his thesis [78], Strömdahl analyzes their work in much detail, while calling our attention to another philosophical problem: as a vast majority of students and teachers understand one mole as the unit measure of number of entities, they adapt a concept that belongs to discontinuum physics, whereas the conventional definition relies on continuum physics.

In a study of 48 first semester college students in the United States, Staver and Lumpe found that students frequently failed to define the mole in terms of carbon-12 and preferentially defined it as a mass or as 'Avogadro number' [69, 80]. Teachers in Spain also exhibited confusion with the concept of the mole and its quantity amount of substance [70]. As in previous studies the mole was most frequently defined as a mass or a number of entities. Similar findings emerged in a study of two chemistry teachers in South Africa [72]. In a 2002 review Furió et al. concluded that great confusion exists among educators and textbooks about the quantity "amount of substance" and its unit the mole [62]. Moreover students reflect this confusion by seldom using "amount of substance" and frequently conceptualizing and using definitions of the mole as a mass or a number ('Avogadro number').

Other researchers have analyzed textbooks used to help students learn chemistry. Furió et al. found in a study of 87 texts used in secondary and university level in Spain published between 1976 and 1996 that the quantity "amount of substance" was not introduced explicitly in 95 % of the analyzed texts [70]. Frequently the mole concept was connected to mass, i.e. molar mass, and to the number of entities. Padilla and Furio-Mas reviewed 30 university level general chemistry textbooks and discovered that 28 out of 30 did not use the current definition of the mole appropriately [71]. Twenty-eight out of 30 describe a mole as being equivalent to the 'Avodgadro number' of entities. Pekdağ and Azizoğlu semantically analyzed 15 chemistry texts with three from the United States, five from France, and seven from Turkey; all were used to teach chemistry at the secondary and university level [73]. This study found similar omissions and mistakes comparable to previous findings where the ”amount of substance” was not used, and the definition of the mole was equivalent to or conflated with molar mass, ‘Avogadro number’, or molar volume. The vast majority of documented teaching practices and textbook descriptions do not support the current SI definition of the unit mole and the quantity amount of substance. This difficulty is consistent with the observed conceptual understanding of both students and teachers about the mole and the amount of substance. As a result, it is unsurprising that a majority of teachers and students define the mole as either a mass or as ‘Avogadro number’.

On a hopeful note some researchers have described pedagogical methods to help teach the concept amount of substance and the mole. Pekdağ and Azizoğlu describe semantic models to help students understand these concepts at the particulate (microscopic), macroscopic, and symbolic levels [73]. The authors suggest that the models could be used as frameworks to guide the development of activities. Fang, Hang, and Clarke [65, 81, 82] developed concept maps to guide the development of activities and to identify relationships between the number aspect and mass aspect of the current SI definition of the mole that they argue need to be made explicit to students. What is lacking in the field is further research to determine the efficacy of these new models in facilitating student learning.

Mills et al. wrote in 2006 ”...it is important that the basis of our measurement system be taught in schools and universities, it is preferable, as far as modern science permits, that the definitions of base units be comprehensible to students in all disciplines, a requirement that becomes increasingly difficult to achieve as science advances” [46]. The proposed re-definition means that the mole is defined as the amount of substance that contains $6.022\,140\,857 \times 10^{23}$ specified entities (using the CODATA 2014 value [3], see also Table 1). Thus, the new definition would achieve Mills’ goal that the definition of base units be comprehensible to students and teachers. In fact, research indicates operationally this is the definition that many teachers, students, and textbooks already use. The goal of a more comprehensible definition is quite likely best achieved by more closely mirroring the practical definition already in use by most students and teachers. This is in contrast to the view expressed in ref. [83] where it is argued that there is no need for a redefinition because the current definition of the mole is well understood and established for almost 50 years.

5.2 The Avogadro constant

In many articles we read that the key concepts used by chemists are not well understood. For example, in the article by Wheatley [84], a widespread divergence of opinion about the nature of the Avogadro constant is shown: some believe it is a number whereas others believe it is a quantity with a dimension of N^{-1}. Peculiar and hard-to-understand to many is also the observation that the Avogadro constant cannot be understood without the mole and yet the proposed definition of the mole rests entirely on the Avogadro constant.

Arguments have also been raised that the Avogadro constant is not a fundamental constant, rather a conversion factor [85]. This view is also shared by Andres et al. [83]. These authors dispute that lack of comprehensibility of the current definition of the mole is an argument for a redefinition, since concepts are well understood for them. The use of quantum metrology is also not considered a valid argument, nor is the dependence of the present definition of the mole on the kilogram an issue, since other dependencies exist in the present SI and will increase in the proposed new SI.

The Avogadro constant is an important tool used by chemists. Following Perrin [21], it guarantees the access to the microscopic reality by tracing the microscopic entity, and even proves the existence of atoms. It is of little value to argue whether a certain concept is 'fundamental' or not as any such discussions will abound with subjective opinions. Ultimately, one cannot forget that all decisions regarding creation and classification of the measurement units are conventions and practical considerations play an important role. Likewise, the CIPM ultimately decided that a philosophical discussion on the nature of the mole was not relevant, the overriding consideration being whether introduction of the mole would serve a useful purpose [22].

Leonard argues [86] that one does not need to involve the Avogadro constant in any SI definition and one could simply define the mole in terms of two units of mass: the kilogram and the atomic unit of mass (dalton, see Note 4 in Table 3). In particular, one has to recognize the 'Avogadro number' which is equal to the gram-to-dalton mass ratio [87] and then stipulate that one mole is the amount of substance which contains the 'Avogadro number' of entities. The proposal by Leonard to explicitly recognize the 'Avogadro number' as the ratio of the gram and the dalton is appealing. A definition of the 'Avogadro number' as being a scaling factor of individual entities was also supported by the IUPAC Analytical Chemistry Division in 2012 [88]. Starting with Eq. (1) to (5) and adding the present definition of the mole [1], it follows that the 'Avogadro number' is the gram divided by the value of the atomic mass unit, m_u, as determined experimentally in gram (of course with an experimental uncertainty). If we change the definition of the mole, as intended in the proposed new SI, so that the 'Avogadro number' is exactly defined, the relation g/m_u is no longer exact but the uncertainty it acquires is negligible. It is easily shown that this follows from Table 3, Line 2 and Eq. (1) to (5), which are unchanged. We also note that the experimental uncertainty of m_u in the proposed new SI will immediately become an order of magnitude smaller than at present.

5.3 Compatibility between molar mass and relative atomic mass ('atomic weight')

Maintenance of compatibility between the molar masses and the relative atomic masses (historically called 'atomic weights') is concerning to some. In short, some authors maintain that chemists appreciate the identity between the numerical values of 'atomic weights' and molar masses [85,89–91]. For example, the molar mass of mercury is $M(\mathrm{Hg}) = 200.592$ g mol^{-1} and the atomic weight of mercury is $A_\mathrm{r}(\mathrm{Hg}) = 200.592$. In the present system of units, mole is defined as the amount of (unbound) carbon-12 atoms in 0.012 kg and dalton is defined as the 1/12 mass of carbon-12 atom. It follows therefore that the molar mass of carbon-12 is 12 g mol^{-1} exactly. In the proposed new SI, however, mole is no longer defined in terms of carbon-12 and consequently there is no stipulation that the molar mass of carbon-12 remains 12 g mol^{-1} exactly. This has the consequence that molar masses are not numerically identical to 'atomic weights' when they are expressed in the SI units of g mol^{-1}, with a difference between the two numerical values currently being less than 1 part in 10^9. Consequently, many contend that the expression relating molar mass and 'atomic weights', $M(\mathrm{X}) = A_\mathrm{r}(\mathrm{X})\, M_\mathrm{u}$ (Eq. (1)) will cease to be used if M_u is no longer 1 g mol^{-1} exactly. This argument can be reformulated by introducing a "correction factor":

$$M(\mathrm{X}) = (1+\kappa)A_\mathrm{r}(\mathrm{X})\, M_\mathrm{u} \tag{17}$$

which allows M_u to remain 1 g mol^{-1} exactly [46]. κ will be zero within to an uncertainty of less than 1 part in 10^9. However, it is also argued that the factor κ is annoying and should be avoided by incorporating it into M_u [86,91,92]. Equation (17) was a suggestion proposed in a 2006 article [46]. The suggestion was subsequently rejected by the CGPM [2] which proposed that, in the new SI, 'the molar mass of carbon-12 $M(^{12}\mathrm{C})$ will be 0.012 kg mol^{-1} but with a relative uncertainty equal to that of the recommended value of $N_\mathrm{A}\, h$ just before redefinition and that subsequently its value will be determined experimentally.' We also find Eq. (17) to be misleading, and even illogical, because Eq. (1) must remain valid in the proposed new SI. See Section 5 of [41] for a simple explanation of how the uncertainty of M_u can be discussed in the same way as the uncertainty of any other experimental quantity if the proposed new SI is adopted.

This Task Group dismisses the concerns in regards to the "incompatibility" between molar masses and 'atomic weights' and has made several observations in this regard. Firstly, important requirements that must be met by a new SI is that the relative atomic mass of carbon-12 keeps its value, $A_\mathrm{r}(^{12}\mathrm{C}) = 12$. Eq. (1) to Eq. (4), which are essential for chemistry, must be unaltered in the proposed new SI. Consequently, the relative uncertainty of the molar mass constant is non-zero, $u_\mathrm{r}(M_\mathrm{u}) \approx 0.45 \times 10^{-9}$ (see Table 3).

Secondly, a discrepancy in the molar mass at the level of 1 part in 10^9 is not in the realm of concern for chemists. The uncertainty in real samples is dominated by impurities [93–95]. To date, the most precise chemical measurement is the measurement of the molar mass of the highly-enriched silicon-28 in the 1 kg single crystal used to determine the value of N_A. This project has been aided by remarkable financial support from the International Avogadro Consortium and, in 2015, the lowest reported relative standard uncertainty of the molar mass of silicon-28 reached 20 parts in 10^9 [96]. Virtually all chemistry measurements operate at precision levels several orders of magnitude worse. In addition, there are only three elements whose standard 'atomic weights' are currently known to a precision below 1 part in 10^9: sodium, fluorine, and phosphorus [40]. Hence, the fact that the molar mass of carbon-12 will now have an uncertainty of less than 1 part in 10^9 can have an impact on the molar masses of only a handful of substances such as F_2, NaF, or PF_3. Last but not least, one cannot forget that the current definition of the mole stipulates that it applies to unbound atoms. Chemists do not work with unbound atoms and binding energy of atoms leads to the loss of mass ($\Delta m = E/c_0^2$). Consequently, the mass of chemical substances does not equal the atomic mass times the number of entities. The molar mass of a crystalline substance X is given by

$$M(\mathrm{X}, \mathrm{cr}) = A_\mathrm{r}(\mathrm{X})\, M_\mathrm{u} - \Delta_\mathrm{f} H_0^0(\mathrm{X})/c_0^2 \tag{18}$$

where $\Delta_\mathrm{f} H_0^0(\mathrm{X})$ is the molar cohesive energy of the crystal at zero kelvin temperature [15] (see Eq. (16)). For a graphite crystal, $\Delta_\mathrm{f} H_0^0(\mathrm{C}, \mathrm{graphite}) = 711$ kJ mol^{-1} which corresponds to a difference between the molar mass of bound and unbound carbon-12, $M(\mathrm{C}, \mathrm{graphite}) - M(\mathrm{C})$, of roughly 7 parts in 10^{10}.

In the current SI, the relative uncertainty of M_u is zero, see Eq. (1). Therefore the error in the calculation of $M(\mathrm{X}, \mathrm{cr})$ is zero only when mass conservation is assumed in chemical reactions. However, conservation of mass is violated at parts in 10^{10}. Thus, one can have identical number of atoms in a gaseous and a solid sample but different masses due to the cohesive energy. This underlines the necessary distinction between the concept of mass and the concept of amount of substance [15].

In summary, currently we are already faced with the numerical incompatibility between molar masses and 'atomic weights' due to binding energy without anyone having an issue with this. Hence, arguing that the "kappa", κ (see Eq. (17)), should be avoided at all costs [86, 91, 92] is unreasonable. In the proposed new SI it will be correct to state that $M_\mathrm{u} = 1$ g mol^{-1}; $u_\mathrm{r}(M_\mathrm{u}) = 0.45 \times 10^{-9}$. The present uncertainty (CODATA 2014 [3]) will in time become an upper limit when more accurate determinations become available. Whereas the current definition of the mole specifies that the carbon-12 atoms referred to in the definition are unbound, at rest and in their ground state, no such specification is needed in the definition of the mole in the proposed new SI.

5.4 Introduction of 'ent' as the amount of a single entity

The current International System of Quantities (ISQ) distinguishes the number of entities B, $N(\mathrm{B})$, and the amount of substance B, $n(\mathrm{B})$, via the Avogadro constant (N_A) as given in Eq. (5). Leonard [86, 92, 97] and De Bièvre [16, 17] have argued repeatedly that it would be better to use the reciprocal of N_A, ent $= N_\mathrm{A}^{-1}$, an amount consisting of a single representative entity, as the particulate unit for amount. It is argued that ”major simplifications in comprehension” results since the following can then be written:

$$n(\mathrm{B}) = N(\mathrm{B}) \cdot \mathrm{ent} \tag{19a}$$

and

$$\mathrm{mol} = \{N_\mathrm{A}\} \cdot \mathrm{ent} \tag{19b}$$

Mole thus can be regarded as the ‘Avogadro number’ of entities instead of the number of the reciprocal Avogadro constant, as it is viewed from the current definition by some [98]. This requires introducing the unit entity, the amount of single entity (symbol: ent), originally proposed in ref. [99], which would be categorized as a unit in use with SI, just like the dalton. Amount of substance would be understood as a number of entities. In other articles, entity was even introduced as the unit of a dimensionless quantity, since atoms, molecules, etc. are discrete objects [100, 101].

From a different point of view, the use of ‘number of entities’ would spoil the achievement gained with the current definition of the mole to resolve the confusion between g-mol and kg-mol [102]; the term ‘amount of substance’ is used to describe a quantity with three conceptually different forms of appearance: chemical mass unit, number of entities and amount of substance.

One could argue that $N = n/\mathrm{ent}$ becomes less comprehensible than $N = N_\mathrm{A}\, n$. Introducing the unit ”entity” would help to clarify that the mole corresponds to the exact number of elementary entities; that is also achieved with the proposed new SI, however. Despite claims to the contrary [97], we note that stoichiometric calculations do not become “more easily comprehended” since in practice stoichiometric calculations do not require the concept of the mole (see Section 2.1).

Furthermore, the scope of a revision of the SI must avoid step changes and unnecessary new names. The revision must be to the benefit of all users. Introducing ‘numerosity’ [103], ‘avo’ [63], ‘ent’ [86, 99], etc. would provoke endless discussions and finding a consensus might be impossible. Alternative names and definitions should only be introduced after broad consultations. The proposed new SI introduces moderate changes, most of which might not even be experienced by the vast majority of users [104].

5.5 Further alternative definitions of the mole

Leonard proposes to redefine the dalton as an exact multiple of the kilogram [97]. Emerson conflates the quantities ‘number of entities’ and ‘amount of substance’ and offers an alternative version of the current definition: ”a mole is a number of elementary entities equal to number of atoms in 0.012 kg of carbon 12”. Emerson also contends that the distinction between n and N is an ”unfortunate result of involving units in definitions of quantities” (for the document, see www.metrologybytes.net/opEds2014.php).

Amount of substance is proportional to a number of entities [1] and understandably many often wonder: ”Why is it then not simply a number of entities?” One can indeed concede that the quantity ‘number of entities’ is logically sufficient and there is no need to introduce a new base quantity ‘amount of substance’ with its own dimension which has led to the definition of the mole and has introduced a new constant: the Avogadro constant. The decision to consider the amount of substance as a quantity with distinct dimension was made in 1971 by the CGPM also in order to facilitate the use of quantity calculus by chemists [19] (and refs. [12,13] cited therein), however the proposal was brought to the CCU jointly by IUPAC, IUPAP, and ISO. Arguments in favor of this decision were recalled in the historical retrospective in Section 2.1 above.

The proposed new SI introduces a change in the definition of mole from a mass basis to a number basis but the practical realization of the mole in a routine laboratory work will still be performed on a mass basis. Consequently, Wheatley finds that the unchanged method to realize the mole demonstrates no practical reason to redefine this unit [84]. He argues that new definitions should only be prompted by better ability to realize the units, which is certainly not the case for the mole. The revised definition of the mole does, however, divorce the concept of amount from the concept of mass. The routine realization of the mole is a procedure based on mass equivalence and has normally a lower precision which is sufficient, however, for many chemical applications, as outlined in Section 5.3 above, and also in Section 5.8 below. Furthermore, as the definition of the mass unit kilogram will change, keeping the old definition cannot be a solution for the problem raised by the author, either. In the New SI this relationship still holds true, however, with a small uncertainty of no practical disadvantage to chemists. Experiments have been proposed to simulate a true realization of the kilogram with very simple means, i.e. with a ’LEGO’ toy watt balance [105], or with a determination of the atomic mass constant from the crystallographic structure of an 20 g aluminium cube, which leads to a value for the Planck constant [106].

Hill et al. [107] compare an ‘electronic kilogram’ (watt balance) and an ‘atomic kilogram’ (based on fixed N_A). The watt balance experiment would lead to more precise electrical measurements but at the expense of introducing a quantum-mechanical current standard. Fixing h would imply that the Planck constant plays a more central role than N_A; chemists might dispute this and the authors suggest to define the kilogram by the mass of $(84\,446\,889)^3 \times 1000/12$ unbound carbon-12 atoms at rest in their electronic ground-state, realized by estimating the number of atoms of silicon-28 in a sphere. The mole would then simply be the amount that contains exactly $(84\,446\,889)^3$ specified elementary entities; the authors believe that this concept is also easily understandable for students. Similar ideas are presented by Khruschov [108] and Si [109]. Both suggest carbon modifications, namely multi-layered graphene [108] or carbon onion structures [109], that is carbon shells around C_{60}, whereas the size of those shells seems to be precisely known. Fox and Hill [110] argue that a perfect cubic structure (fcc) of carbon-12 would need only one length to be described, in contrast to rectangular and parallelpiped or a spherical structure. Neither of these proposals have any scientific merit as they rely on imagined and yet unrealized molecular structures. Other proposals have been put forward to remedy this apparent pedagogical problem. We have the binary mole (2^{79}, accurate to two digits), the empirical mole ($23! \times (23 + \sqrt{2/23})$, accurate to four digits), and the cubic mole ($84\,446\,889^3$, accurate to seven digits). Given that the latter is a simple and accurate representation of the current best estimate of $\{N_\mathrm{A}\}$, one could indeed concede that stipulating $\{N_\mathrm{A}\} = 84\,446\,885^3$ (accurate to eight digits) is perhaps a better way to define the mole [110].

It was criticized that the current definition of the mole lists the nature of the elementary entities. The term ‘elementary’ should be replaced by ‘of the same kind’ [111]. Furthermore, the definition of the mole should not have the same structure as the other four revised base units in the proposed new SI, since the mole has a different status in physics [111].

5.6 On the circularity of the current definition of the mole

Many have asserted that the current definition of the mole is a seemingly circular definition [16]. When rewritten in an explicit constant version, it takes the following form:

> The mole is the unit of amount of substance. It is defined by taking the fixed numerical value of the molar mass of carbon-12 to be 0.012 when expressed in the unit kilogram per mole, where the kilogram has already been defined.

This definition of the mole appears to be circular because the definition of molar mass (mass of one mole of substance) is assumed *a priori*. The circularity is illusory and is only due to giving the name ‘molar mass’ to the quantity $M = m/n$, an unfortunate example of conflating names of quantities and units [11]. If this quantity had been called ‘mass-to-amount ratio’, the complaints regarding circularity would likely disappear.

In addition, the definition of the Avogadro constant can be derived from the definition of the mole without any circularities. There are three ISQ equations that are pertinent to understanding any definition of the mole:

$$n(\mathrm{X}) = N(\mathrm{X})/N_\mathrm{A}$$

This equation is identical with Eq. (5).

$$m(\mathrm{X}) = N(\mathrm{X})\, m_{\mathrm{a}}(\mathrm{X}) \tag{20a}$$

$$M(\mathrm{X}) = m(\mathrm{X})/n(\mathrm{X}) \tag{20b}$$

Using only the information that the mole is the unit of amount of substance, the first equation tells us that $n(\mathrm{X}) = 1$ mol when $N(\mathrm{X}) = \{N_{\mathrm{A}}\}$. By combining the three equations, the definition of the mole as stated above also tells us that if X is ^{12}C, then $n(^{12}\mathrm{C})$ $= 1$ mol when $N(^{12}\mathrm{C}) = \{N_{\mathrm{A}}\} = 0.012$ kg$/m_{\mathrm{a}}(^{12}\mathrm{C}) = 0.001$ kg Da^{-1}. Thus pedagogues who teach that the numerical value of the Avogadro constant is the ratio of the gram to the dalton expressed in gram are being consistent with the present definition of the mole.

5.7 Name of the quantity

In 2009, ICTNS indicated that the name ”amount of substance has been a source of much confusion and that the greatest effort should be made to change the name ... at the same time that a new definition of the mole is approved” [33]. Likewise, the quantity name ‘amount of substance’ has been criticized as ”not well chosen” [112] and ”is practically unknown to most teachers” [70]. Leonard argues that the name for the base quantity should be ‘chemical amount’, by analogy with ‘electric current’ [113]. In fact, ‘chemical amount’ had appeared as the alternative name for ‘amount of substance’ in the IUPAC Green Book since 1993 [114]. It has also been said that the name of the quantity ‘amount of substance’ is too long and should be replaced, for instance by ’numerosity’ [103], by ’ment’ [18], or by ’enplethy’ [115].

As mentioned in Section 5.4, the scope of a revision of the SI must avoid step changes and unnecessary new names. This Task Group therefore concluded that the name ‘chemical amount’ should be preferred. When there is relevant chemical context, one can also talk about the chemical amount of photons or chemical amount of electrons.

5.8 Metrological aspects

More and more laboratories are currently being equipped with the experimental tools of either of the two available experimental protocols to realize the kilogram [38, 39, 116]. Concern was raised that only a few countries in the world will be capable of affording the realization of the kg in the proposed new SI [49]. In the meantime, the groups from NRC and NIST have reported excellent uncertainties using Kibble watt balances, 1.5 parts and 3.4 parts in 10^8 respectively. NIST expects a further reduction in their uncertainty by July 2017. An additional five groups anticipate substantial progress in the near term with their own Kibble watt balances. Several other laboratories are in earlier stages of development [116]. PTB (Germany) intends to supply primary silicon spheres to laboratories who may wish to buy them and less expensive secondary standards made of natural single-crystal silicon. They will also provide 'service after sale' to keep the primary standards primary and to recalibrate the secondary standards. It seems, however, even a situation envisioned in [49] was considered to be acceptable by the CCM experts in mass metrology [37].

A comprehensive treatise on the subject of redefinition providing desirable qualities for the definition of a unit has been put forward [102,117], with qualities for the definition of base units as follows: definitions should be simple and freely available to everyone; standards should be related to stable 'invariants of nature'; realization of the definitions must be reproduceable and of high precision (best measurements), if precision increases, revising the definitions should be made possible [117].

Traceability within the SI ensures that measurement results are comparable toconsistent with results from different measurement methods. As implied in [102, 118] a primary (direct) method of measurement guarantees highest metrological quality. It is accepted without reference to a standard measuring the same quantity.

What is appealing to some metrologists is that in the proposed new SI, the uncertainties for the atomic and the molar mass constant become identical once N_A is fixed, see Eq. (4) [94,95,119].

Chemical measurements do depend on a realization of the mole through a primary (direct) method of measurement [102, 118]. The mole, however, does not depend on a particular method of realization. The use of a primary (direct) method of measurement is important to realize the unit at a high standard, but various secondary methods of realization can be devised. Weighing a sample of material with known purity (and therefore known relative molar mass), for instance, is used to determine the amount of substance

$$n(\mathrm{X}) = \frac{m(\mathrm{X})}{A_\mathrm{r}(\mathrm{X})\, M_\mathrm{u}} \tag{21}$$

and this would be unchanged in the proposed new SI [94]. In Eq. (21), $m(\mathrm{X})$ is the mass of a sample of entity X corrected for impurities; the molar mass constant M_u would have an uncertainty in the proposed new SI. As discussed in Section 5.3 above, the change to the experimental accuracy is entirely negligible as explained in Section 5 of [41]. This argument should alleviate the anxiety expressed in [89].

If one could instead determine the number of entities $N(\mathrm{X})$ of X using a primary method, the amount of substance would be given by Eq. (5), $n(\mathrm{X}) = N(\mathrm{X})/N_\mathrm{A}$, and the amount of substance that corresponds to a single entity X ($N(\mathrm{X}) = 1$) would be $n(\mathrm{X}) = N_\mathrm{A}^{-1}$

exactly, where N_A is the Avogadro constant [119].

The silicon XRCD experiment that can be used to realize the kilogram in the proposed new SI [39] also realizes the value of $n(^{28}\mathrm{Si})$ to very high accuracy with no weighing involved [41]. Weighing the silicon sphere will give the same result at potentially the same accuracy using Eq. (21). The uncertainty of M_u in the proposed new SI is completely negligible even in this extreme case.

6 Questionnaire

The letter to NAOs was sent out in June 2014 to the official representatives of IUPAC National Adhering Organizations (NAOs) using email addresses as they appear on iupac.org. The announcement of this activity was published in the official IUPAC news magazine in July 2014 [120] and in September 2014 [121]. In addition, an announcement of this consultation also appeared in August 2014 in the journal Accreditation and Quality Assurance [122], an announcement of this action was posted on the IUPAC NAO forum of the IUPAC Discussion Board (at forum.iupac.org) by the IUPAC Secretariat (10 July 2014).

In this letter, all the NAOs were asked to answer in written form to the below listed questions and return their document no later than 2014-10-01.

QUESTIONNAIRE
IUPAC NAOs are hereby asked the following:

1. Are you (as NAO representing your members) satisfied with the current definition of the mole?
   (a) YES or NO?
   (b) If NO, please specify in a few sentences why you opted for NO.
   (c) If NO, please provide some suggestion on what to change.
2. Are you (as NAO representing your members) satisfied with the new definition of the mole as proposed by the 24th General Conference of Weights and Measures?
   (a) YES or NO?
   (b) If NO, please specify in a few sentences why you opted for NO.
   (c) If NO, please provide some suggestion on what to change.
3. Are you (as NAO representing your members) satisfied with the current definition of the quantity amount of substance?
   (a) YES or NO?
   (b) If NO, please specify in a few sentences why you opted for NO.
   (c) If NO, please provide some suggestion on what to change.
4. Are you (as NAO representing your members) satisfied with the current name of the quantity amount of substance?
   (a) YES or NO?

(b) If NO, please specify in a few sentences why you opted for NO.

(c) If NO, please provide a suggestion for a new name.

The responses from the following twenty countries were received : Australia, Belgium, Brazil, Canada, Egypt, France, Great Britain, Greece, Hungary, Ireland, Italy, Nepal, Netherlands, Norway, Portugal, Slovakia, Slovenia, United Kingdom, United States of America, and Uruguay.

Summaries of all answers are listed in the following Table 4. Some NAOs answered very short, others wrote helpful comments. All answers are available at full length as PDF on the IUPAC webpage for download [6]. Inspection of the table shows that the replies from the NAOs were diverse rather than tending to any unified opinion either on the proposed definition of the mole or in regard to the current definition or the name of the quantity ‘amount of substance’.

Table 4: Answers received to the questionnaire which have been mailed to all the IUPAC NAOs and their respective summarized answers to the four questions.

Country	1971 unit definition *Q1*	2014 unit definition *Q2*	quantity definition *Q3*	quantity name *Q4*
Australia	YES	YES	YES	NO
Belgium	NO	NO	NO	NO
Brazil	NO	NO	NO	NO
Canada	YES	NO	YES	YES
Egypt	YES	–	YES	YES
France	YES	NO	YES	YES
Great Britain	NO	YES	YES	YES
Greece	NO	YES	NO	YES
Hungary	NO	YES	NO	NO
Ireland	NO	YES	NO	YES
Italy	NO	NO	NO	NO
Nepal	YES	YES	YES	YES
Netherlands	NO	NO	–	NO
Norway	–	YES	–	–
Portugal	NO	YES	YES	NO
Slovakia	NO	YES	YES	YES
Slovenia	–	–	–	–
Uruguay	YES	YES	YES	YES
USA	NO	NO	NO	NO
Total YES	6	10	9	9
Total NO	11	7	7	8

Some IUPAC members and international organizations felt that the questionnaire was being used as a vote on the matter, which was not its aim. The purpose of the questionnaire was simply, however, ”to collect opinions and comments”, if any, by the NAOs of IUPAC and this was clearly stated in the cover letter.

The total count at the bottom of this table shows that a majority is not satisfied with the current definition of the unit mole. A slight majority is in favour of the new definition as being proposed in the new SI [2]. As far as the definition of the quantity amount of substance and its name are concerned, there seems to be no clear position. From the answers to four questions raised, there was no emerging consensus on the definition of the mole. Opinion on all questions was, in fact, equally divided.

Despite the diversity of ’yes’ and ’no’ answers, the detailed replies show unambiguously that there is a need for a better formulation of what is ‘amount of substance’. Many replies also raised numerous technical issues the treatment of which are beyond the scope of this project. The full detail of the answers will be made public at the aforementioned web site of the minutes of the Task Group meeting in Ottawa, in January 2015 [6].

7 Conclusions

7.1 Conclusions on the definition of the mole

The contents of this manuscript are the result of a Task Group work commanded by three divisions of the International Union of Pure and Applied Chemistry, IUPAC (Divisions I, II and V), as well as by IUPAC's Interdivisional Committee on Terminology, Nomenclature and Symbols, ICTNS, and IUPAC's Commission for Chemical Education, CCE. The aim of this work was the preparation of a text containing a summary of facts and opinions about two imminent changes in the International System of units, SI: the new definition of the kilogram and that of the mole [2]. Further to this, a critical assessment of these facts and opinions should be made, where appropriate and convenient.

More than 100 published contributions related to this matter were read, carefully analyzed and discussed. Additionally, a poll survey was launched among national adhering organizations (NAO) of IUPAC. The Task Group concluded that that the proposed new definitions have been studied sufficiently well to be successfully implemented. The opinions expressed by members from educational and metrological scientific communities, as well as by scientists practicing chemistry hold that the new definitions are needed and are even highly desirable. A careful analysis has shown that a remaining reticence among some chemists with respect to the new definition of the mole is not justified, either in concern over accuracy issues, or in reference to routine work in a chemical laboratory. A majority of opinions from the published material analyzed in this work were in accord with the results from the questionnaire study.

Based on its own critical work, the Task Group naturally developed its own consolidated position with respect to the mole. This position is formulated as an epilogue, and appended to this manuscript. It might be of help to IUPAC to review the position of the Union with respect to the proposed new SI.

7.2 Conclusions on the name of the quantity

In the educational literature there is confusion among students, teachers, and textbook authors regarding the term 'amount of substance'. Also the poll evaluation carried out during this work proves that many IUPAC NAOs are not satisfied with the current formal definition of the quantity 'amount of substance'. Pursuant to the 2009 recommendation of ICTNS to the IUPAC Bureau [33], this Task Group discussed a suitable alternative name for the amount of substance. A discussion arose regarding many proposed names for the quantity. Based on the papers reviewed in this work, it seems that the name 'chemical amount' would be the best choice and that the concept would also be useful when no chemical substances are involved.

As some authors have reflected, the name ‘chemical amount’ has an analogy to ‘electrical current’. Many have criticized the name amount of substance largely on the basis that it is a three-word name. However, this is a widespread misunderstanding in regards to the use of the name amount of substance. The IUPAC Green Book (3rd edition) points out that ”the words of substance may be replaced by the specification of the entity” (see Section 2.10 [11]). Hence, in practice we speak of amount of oxygen and not amount-of-substance of oxygen. In that sense, ‘substance’ in ‘amount of substance’ is a placeholder name and ‘chemical amount’ might avoid this misunderstanding. In addition, the adjective ‘chemical’ can be omitted when sufficient context permits much like the name ‘electrical current’ is often shortened to ‘current’ in the scientific literature.

Examples

chemical amount of dioxygen is 5 mol, $n(\mathrm{O_2}) = 5$ mol
chemical amount of iron(III) oxide is 2 mol, $n(\mathrm{Fe_2O_3}) = 2$ mol
amount of dioxygen is 5 mol, $n(\mathrm{O_2}) = 5$ mol
amount of iron(III) oxide is 2 mol, $n(\mathrm{Fe_2O_3}) = 2$ mol

In fact, ‘chemical amount’ has appeared as an alternative name for ‘amount of substance’ in the IUPAC Green Book since 1993 [114]. This Task Group concluded that the name ‘chemical amount’ might be the preferred name among all names suggested so far. When there is relevant chemical context, one can also talk about the chemical amount of photons or the chemical amount of electrons. However, amount of photons and amount of electrons are sufficiently well understandable expressions. We finally note that the task of formulating a recommendation for a new name for the quantity amount of substance was outside the scope of the present IUPAC Technical Report. Our work might nevertheless serve as a basis for a future thorough discussion about this specific question within IUPAC.

8 Acknowledgements

This work has benefited from fruitful discussions with many bodies and members of IUPAC and outside the Union. In particular, we thank Professor Ian Mills, Dr. Franco Pavese and Dr. Barry Wood for numerous exchanges on this matter. We also thank the National Research Council of Canada for the hospitality during our Ottawa meeting. We gratefully remember the late Professor Paul De Bièvre, who inspired many of us with his enthusiasm and critical view on this matter.

Epilogue

During several intense discussions conducted by this Task Group in the context of the present work, the following text emerged as an honest union of converging opinions. It contains a proposal, by this Task Group, of a new wording for the definition of the mole and in that it reflects the 2009 ICTNS final motion that the quantity amount of substance should also be renamed.

> The chemical amount, n, is a measure of the number of specified elementary entities. An elementary entity may be an atom, a molecule, an ion, an electron, any other particle or specified group of particles. The mole, symbol mol, is the SI unit of chemical amount. One mole contains exactly $6.022\,140\,857 \times 10^{23}$ elementary entities. This number of elementary entities is called the Avogadro number.
>
> Further specifications:
>
> (1) The chemical amount of a substance B, $n(\mathrm{B})$, is proportional to the number of entities of B, $N(\mathrm{B})$, with
>
> $$n(\mathrm{B}) = N_\mathrm{A}^{-1}\, N(\mathrm{B})$$
>
> The proportionality factor is a universal physical constant that is independent of the nature of the substance. Its reciprocal, N_A, is the Avogadro constant which is the same for all substances.
>
> (2) The stipulated Avogadro number $\{N_\mathrm{A}\} = 6\,022\,140\,857 \times 10^{14}$, will be the numerical value of the Avogadro constant, $N_\mathrm{A} = 6.022\,140\,857 \times 10^{23}\ \mathrm{mol}^{-1}$. The Avogadro constant has the SI unit mol^{-1}, because the chemical amount n is a base quantity with the SI unit mol and because the number of entities, being a number, is a quantity of dimension one (i.e. dimensionless).
>
> (3) The chemical amount of B, $n(\mathrm{B})$, is also proportional to the mass of B, $m(\mathrm{B})$, with
>
> $$n(\mathrm{B}) = M(\mathrm{B})^{-1}\, m(\mathrm{B})$$
>
> The proportionality factor is the reciprocal of the molar mass, $M(\mathrm{B})$, which is a characteristic constant of the substance B.
>
> (4) The previous definition of the mole implied that the Avogadro number is the ratio of the gram to the dalton, with the value of the dalton expressed

in gram. The historical continuity of the present definition preserves this relation to within an uncertainty negligible for practical purposes.

A few remarks:

The molar mass of any atom or molecule B, $M(\mathrm{B})$, may still be obtained from its relative atomic mass (”atomic weight”), $A_\mathrm{r}(\mathrm{B})$, from the equation

$$M(\mathrm{B}) = A_\mathrm{r}(\mathrm{B})\, M(^{12}\mathrm{C})/12 = A_\mathrm{r}(\mathrm{B})\, M_\mathrm{u}$$

In this equation M_u is the molar mass constant, equal to $M(^{12}\mathrm{C})/12$. Because the molar mass of unbound carbon-12, $M(^{12}\mathrm{C})$, is no longer 12 g mol^{-1} exactly, the molar mass constant, M_u, is no longer 1 g mol^{-1} exactly. Its uncertainty, however, is of no practical relevance in chemistry, being smaller than 1 part in 10^9. Within this uncertainty, the value of M_u remains 1 g mol^{-1}. The molar mass of any atom or molecule B is also related to the mass of the elementary entity, $m(\mathrm{B})$, by the equation

$$M(\mathrm{B}) = N_\mathrm{A}\, m(\mathrm{B}) = N_\mathrm{A}\, A_\mathrm{r}(\mathrm{B})\, m_\mathrm{u}$$

and m_u is the atomic mass constant equal to $m_\mathrm{a}(^{12}\mathrm{C})/12$. M_u and m_u are related with the Avogadro constant through the equation

$$M_\mathrm{u} = N_\mathrm{A}\, m_\mathrm{u}.$$

Appendix – Definition of the kilogram based on the Planck constant

The kilogram, symbol kg, is the SI unit of mass; its magnitude is set by fixing the numerical value of the Planck constant. The proposed new SI sets the numerical value of the Planck constant, symbol $\{h\}$, to exactly $6.626069\text{Y}\times10^{-34}$ when expressed in the SI unit for action J s = kg m^2 s^{-1} thereby defining its magnitude (the final missing digits abbreviated by Y are still being determined). Thus, in the proposed new SI the same experiments that are currently able to determine the value of the Planck constant will become the primary means to realize the new definition of the kilogram based on the fixed numerical value for h. Two kinds of such experiments are currently persued and we give here a short summary of the main ideas linking the Planck constant h to the kilogram.

Crystal density approach or atom counting

The h-based definition of the kilogram can be realized by what is known as the crystal density approach (also known as the atom counting) which relies on the fact that the density of a perfect macroscopic crystal with mass m and volume V is the same as the ratio of mass to volume of its atomic-scale unit cell:

$$\frac{m}{V} = k\,\frac{m_{\rm a}({\rm X})}{V_{\rm a}} \tag{22}$$

The crystal is composed of the chemical element X whose atomic mass is $m_{\rm a}({\rm X})$. The volume $V_{\rm a}$ of each unit cell contains exactly k atoms (for example, if X is silicon, then $k = 8$ the unit cell of silicon is a face-centred, diamond-cubic structure which is the building-block of defect-free, ultra-pure silicon monocrystals). The number of atoms in the crystal equals $N = m/m_{\rm a}({\rm X})$. Following Eq. (22), N can be determined from

$$N = k\,\frac{V}{V_{\rm a}} \tag{23}$$

where k is known exactly whereas V and $V_{\rm a}$ can be determined to high accuracy by optical interferometry and X-ray interferometry, respectively. Thus,

$$m = N\,m_{\rm a}({\rm X}) = N\,A_{\rm r}({\rm X})\,m_{\rm u} \tag{24}$$

$m_{\rm u}$ is the atomic mass constant, $12\,m_{\rm u} = m_{\rm a}(^{12}{\rm C})$, which has the SI unit kg, and $A_{\rm r}({\rm X})$ is the relative atomic mass ('atomic weight') of X, which is of dimension one (i.e. dimensionless), as is N. Multiplying the right-hand side of Eq. (24) by $1 = h/h$ results in

$$m = h\,N\,\frac{m_{\rm a}({\rm X})}{h} = h\,N\,A_{\rm r}({\rm X})\,\frac{m_{\rm u}}{h} \tag{25}$$

The quantity $m_{\rm u}/h$ is a physical constant with the SI unit m^{-2} s. It has been measured to high accuracy in two different types of atomic-physics experiments [42,43]. In fact, the relative uncertainty of m_{u}/h is far smaller than the relative uncertainty (parts in 10^8) to which N can presently be determined.

Thus, if one can produce a pure crystalline substance of suitable size and shape, it is possible to calculate its mass in kilogram traceable to a fixed value of the Planck constant h [106]. The crystal can then be used as a primary mass standard to disseminate the SI unit of mass to secondary standards.

Kibble balance (Watt balance)

The h-based definition of the kilogram can be realized by a second kind of experiments that relies on comparing electrical power to mechanical power (see for example [123]), which is popularized in a form of a LEGO watt-balance [105] or a loudspeaker-based balance [124].

Consider a horizontal wire carrying an electric current I. If a length L of the wire is in a horizontal magnetic field of flux density B oriented perpendicular to the flow of the current, the Lorentz force F on the wire will be vertical and is given by

$$F = B\,L\,I \tag{26}$$

In an appropriate geometry, of which there are many, F can be made to compensate the weight $G = m\,g$ of an object of mass m, where g is the acceleration of gravity at the position of the object. At equilibrium,

$$m\,g = B\,L\,I \tag{27}$$

This is the principle behind the operation of a modern analytical balance, but the balance response, $I(BL/g)$, is displayed as a unit of mass simply by calibrating the balance with a standard whose mass is traceable to the international prototype kilogram (IPK).
The Kibble balance eliminates the term BL by a second measurement: The same wire is made to move vertically with velocity v, which causes a tension U to be induced between the ends of the wire. Under these conditions,

$$U = B\,L\,v \tag{28}$$

Eliminating BL from Eq. (27),

$$m\,g\,v = U\,I \tag{29}$$

where the left side of Eq. (29) is a virtual mechanical power and the right side is a virtual electrical power; hence the earlier name Watt balance, after the SI unit of power. The power in both cases is "virtual" because it is derived by combining results from two different operations, neither one of which involving power generation or loss.
By measuring I in Eq. (29) from Ohm's law, $U' = R\,I$,

$$m = \frac{U\,U'}{g\,v\,R} \tag{30}$$

To determine the mass m to the highest accuracy and at the same to introduce h, all five quantities on the right side of Eq. (30) must be measured as accurately as possible. By eliminating the current I, the electrical quantities can be measured in terms of quantum standards commonly used to obtain maximum precision in resistance [125] and tension (voltage) [126] metrology. This also introduces h to the right side of Eq. (30), which is the goal. The quantum standards are based on the quantum Hall effect, first reported in 1980 by von Klitzing et al. [127] and the AC Josephson effect, first predicted and then observed in 1962/1963 [128, 129]. Both have been perfected over the ensuing years. The AC Josephson effect provides ideal frequency-to-tension conversion, described by

$$U_n = n\, f\, \frac{h}{2e} \tag{31}$$

where e is the elementary charge, h is the Planck constant and f is the frequency of microwaves which irradiate the two weakly coupled superconductors that form the circuit element. The unit of h/e is V/Hz. The characteristic curve of observed tension across the junction as a function of applied current passing through the circuit reveals quantized "steps" in the tension. The height of each step is $hf/2e$ and the stable tension of the n-th step is given by Eq. (31).

The quantum-Hall effect was first observed in semiconductors, where a test sample has a width that is much greater than its thickness but much less than its length. At cryogenic temperature, and in the presence of a strong magnetic field perpendicular to the length-width surface, a constant current flowing along the length of the sample will create a tension, the "Hall voltage", perpendicular to both the current and the magnetic field, i.e. across the width of the sample. The ratio of the Hall tension ('voltage') to the current is the Hall resistance R_{H}. Constant values of R_{H} are observed as a function of increasing magnetic flux density. These "plateaus" are described by

$$R_{\mathrm{H}} = \frac{1}{i}\,\frac{h}{e^2} \tag{32}$$

where i is the integer defining the i-th plateau. The value of i decreases as the applied magnetic flux density increases. The quantity h/e^2 is a quantum of resistance, equal to about 26 kΩ, which is the resistance of the highest possible plateau ($i = 1$).

Finally, apart from some manageable details discussed in [123], Eq. (30) becomes

$$m = h \left(\frac{n\, n'\, i}{4}\right) \frac{f\, f'}{g\, v} \tag{33}$$

where m will be determined from the fixed value of h, a collection of exact integers, two frequencies, a velocity and the acceleration of gravity. Note that e does not appear in Eq. (33), which means that a value of e is superfluous to this method. Exact values of both e and h are, of course, needed for electrical metrology based on $h/2e$ and h/e^2. Simplified presentations can be found in [105, 124], with a deeper analysis in [123].

Acronyms

This paragraph contains a list of acronmys used in the preceeding text together with their english or (when applicable) french translation.

Acronym	English/French
BIPM	International Bureau of Weights and Measures / Bureau International des Poids et Mesures
CCU	Consultative Committee on Units / Comité Consultatif des Unités
CGPM	General Conference on Weights and Measures / Conférence Générale des Poids et Mesures
CIPM	International Committee for Weights and Measures / Comité International des Poids et Mesures
CODATA	Committee on Data for Science and Technology
ICTNS	Interdivisional Committee on Terminology, Nomenclature and Symbols
IPK	international prototype kilogram
ISO	International Organization for Standardization
ISQ	International System of Quantities
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics
NAO	National Adhering Organizations
PDF	portable document format
SI	International System of Units / Système International d'Unités
XRCD	X-ray crystal density

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