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The Background and Implications of the "New SI" for Analytical Chemists

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Summary

The International System of Units (SI) is not in itself a complete philosophical system; it has been developed over time to deal with practical needs. It started during the French revolution with units of unified length and mass. By the mid-1800's three base units were in place, for measuring distance, mass and time (centimetre, gram and second, the CGS system). These base units evolved into the metre, kilogram and second (the MKS system). The ampere became the fourth base unit in 1946. In 1954 the kelvin and the candela were added as new base units. Finally, in 1971, the mole became the seventh base unit, for the amount of substance[1,2]*. The definitions of each base unit have undergone continuous evolution to deal with improvements in measuring capabilities and following the realisation of any shortcomings in the prior definitions.*

The revision presently on the way will lead to the "New SI" that again comprises of seven base units, namely the second, s; the metre, m; the kilogram, kg; the ampere, A; the kelvin, K; the mole, mol and the candela, cd[3]*.*

From the Present SI to the New SI

The "weak" element in the present SI system is the kilogram, which is defined by an artefact, the international prototype of the kilogram (IPK). This is a cylinder made of an alloy in which the mass fraction of platinum is 90 % and the mass fraction of iridium is 10 %, cast in 1879 by Johnson Matthey, and kept in air under three bell jars at the International Bureau for Weights and Measures (BIPM) in a vault in Sèvres (Paris, France). Three comparisons have been carried out between the IPK and the official copies stored under different conditions at BIPM, the most recent being in 1989. These comparisons show a trend towards larger average mass of the copies with respect to the IPK of approximately 50 µg over 100 years[4,5]. These small changes are thought to be due to contamination from atmospheric mercury and the growth of a carbonaceous layer, the latter can be removed by UV/ozone treatment[6]. Such drifts go unnoticed among the typical uncertainties of mass measurements in analytical chemistry laboratories. The same holds for the ampere and mole (as well as for the candela) whose definitions depend on the kilogram; however these small drifts do not go unnoticed in other areas, such as quantum and nuclear physics and astronomy.

In addition to the kilogram problem, the definition of ampere became considered to be old-fashioned, based on the force between two wires, rather than a charge flow as used in everyday practice and in electrical metrology. Although the candela could be dispensed with it will continue as it is so enmeshed in its special applications of photometry and radiometry for industrial use and in the environmental field[7,8]. Thus, for the reasons given above it was considered by BIPM desirable to update the whole system[9].

A proposal for such an update has been prepared by the Consultative Committee on Units (CCU), which reports to the International Committee for Weights and Measures (CIPM) who produce the necessary resolutions for consideration and eventual decision by the General Conference on Weights and Measures (CGPM) of the BIPM acting under the Metre Convention[1].

The case for the proposed new system has been debated, mainly positively, in a series of papers in *Meterologia*[9-14] and in papers presented at the Royal Society Discussion Meeting – The New SI Based on Fundamental Constants, 24-25 January 2011[15].This discussion was designed to follow on from the earlier Royal Society meeting – The Fundamental Constants of Physics, Precision Measurements and the Base Units of the SI", held 14-15 February 2005[16].

The International Union of Pure and Applied Chemistry (IUPAC) position, the custodian of the International Table of Atomic weights, is as stated by J. Lorimer in the *post scriptum* to his article "Old Concepts and New" as follows:

> *"On behalf of the Bureau, the IUPAC Executive Committee at its meeting 2 October 2009 reviewed and accepted the ICTNS recommendations to support the mole as proposed by the CCU"*[17]

ICTNS is the IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols.

The IUPAC has informed of the impending change to the SI in a series of articles in *Chemistry International*, in the main they promote the New SI[18-23]. Discussions, particularly in the journal *Accreditation and Quality Assurance*, indicate that not all chemists and engineers are happy with the proposed changes to the SI[24-33]. Given that the decision to adopt the New SI is in effect a *fait accompli*, due to the authority vested in the BIPM set up by the Metre Convention of 1875 and amended in 1921[1], those affected will have to adapt to live with the new system.

In this article are outlined the basic aspects of the New SI system that affects chemistry, its advantages and the problems with which chemists will have to deal, specifically with regard to the kilogram and the mole, in day to day practice and also when teaching new entrants to the profession.

What is New about the "New SI"?

The revision of the SI system has given the opportunity to reinforce the basis of the system. The idea was to go from measurable artefacts to defined, "universal" or "fundamental" constants of nature, those which according to current knowledge seem not to change in time and space. If in reality they are strictly constant they would be the ideal anchor points for a Unit System. A set of seven constants was chosen for reference.

So far the values of these constants have been measured and monitored. As they are considered by CCU neither to depend on where they are measured nor show a measurable drift, their values will be fixed according to the "best estimate" derived from all appropriate measurement results and codified. At least at the time of fixing there will be no discrepancy – a sort of a snapshot of reality – and, if truly invariant, also not in the future. The constants that will comprise the New SI are (units and their symbols are defined in the lower list):

- the hyperfine splitting frequency of the caesium-133 atom in ground state and rest at zero thermodynamic temperature, $\Delta\upsilon\ (^{133}\mathrm{Cs})_{\mathrm{hfs}}$, is exactly 9 192 631 770 Hz
- the speed of light in vacuum, *c*, is exactly 299 792 458 m s^{-1}
- the Planck constant, *h*, is exactly $6.626\ 069\mathrm{X}\times10^{-34}$ J s
- the elementary charge, *e*, is exactly $1.602\ 176\mathrm{X}\times10^{-19}$ A s
- the Boltzmann constant, *k*, is exactly $1.380\ 648\mathrm{X}\times10^{-23}$ J K^{-1}
- the Avogadro constant, $N_{\mathrm{A},}$ is exactly $6.022\ 141\mathrm{X}\times10^{23}$ mol^{-1}
- the luminous efficiency, K_{cd}, of monochromatic radiation of frequency 540×10^{12} Hz is exactly 683 lm W^{-1}

The symbol X represents the additional digits to be added to the numerical values of *h*, *e*, *k* and N_A according the state of knowledge at the time that these revised definitions and the revised text for Chapter 2 of the SI Brochure are finally adopted[3].

The seven base units of the new system are derived from these constants using their values and well-known physical relationships and in outline are as follows:

- the second, s, unit of time, is based on the frequency of the radiation related to $^{133}\mathrm{Cs}$ hyperfine splitting, $\Delta\upsilon(^{133}\mathrm{Cs})_{\mathrm{hfs}}$
- the metre, m, unit of length, is based on the speed of light *c* and the unit s
- the kilogram, kg, unit of mass, is based on the Planck constant *h*, the speed of light *c* and the unit s
- the ampere, A, unit of electric current, is based on elementary charge *e* and the unit s
- the kelvin, K, unit of thermodynamic temperature, is based on Boltzmann constant *k* and the (derived) unit joule, $\mathrm{J} = \mathrm{s}^{-2}\ \mathrm{m}^2\ \mathrm{kg}$
- the mole, mol, unit of amount of substance is based on Avogadro constant, N_{A}
- the candela, cd, the unit of luminous intensity, is based on the luminous efficacy K_{cd} of radiation of 540 THz and the unit watt, $\mathrm{W} = \mathrm{s}^{-3}\ \mathrm{m}^2\ \mathrm{kg}$

The sequence of the entries of this list is chosen in such a way that for each given unit those units necessary to define it have been introduced before it.

Definitions of the New SI Units of Particular Importance in Everyday Life and for Analytical Chemists

In everyday life the most used units are those for time interval, the second, for distance, the metre and for mass, the kilogram; additionally for chemists, the mole is of major importance.

The current and previous systems of units were based on "explicit-unit" definitions, i.e. their values were defined and thus units carry no measurement uncertainty – a distinction which is made obvious by writing their symbols with Roman font (upright) rather than in italic style (tilted) as are symbols of quantities and reference values.

The New SI system is stated in terms of "explicit-constant" definitions in which the reference constant will be attributed an exact **numerical** value[2] according to the best knowledge at the moment the New SI is released into effect, after that the units serve to guarantee the value of the constant. The proposed definitions are as follows:

The Second, Unit of Time[3]

The second, s, is the SI unit of time; its magnitude is set by fixing the numerical value of the ground-state hyperfine splitting frequency of the caesium-133 atom, at rest and at zero thermodynamic temperature, to be equal exactly to 9 192 631 770 when expressed in the unit s^{-1}, which is equal to Hz.

Thus, we have the exact relation:

$$\Delta \upsilon(^{133}\mathrm{Cs})_{\mathrm{hfs}} = 9\ 192\ 631\ 770\ \mathrm{Hz}$$

The effect of this definition is that the second is the duration of exactly 9 912 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium-133 atom.

From the above equation one arrives at

$$\mathrm{Hz} = \Delta \upsilon(^{133}\mathrm{Cs})_{\mathrm{hfs}} / 9\ 192\ 631\ 770$$

The use of "Hz" in this equation, rather than "1 Hz", illustrates the confusion noted earlier[26] as the "Hz" implies it is a quantity.

To be explicit as to "what is a second?" the equation needs to be rearranged to give:

$$\mathrm{s} = 9\ 192\ 631\ 770\ /\ \Delta \upsilon(^{133}\mathrm{Cs})_{\mathrm{hfs}}$$

which is equivalent to the current SI unit for interval of time.

The Metre, Unit of Length[3]

The metre, m, is the SI unit of length; its magnitude is set by fixing the numerical value of the speed of light in vacuum to be equal to exactly 299 792 458 when it is expressed in units of $\mathrm{m\ s^{-1}}$.

Thus, we have the exact relation

$$c = 299\ 792\ 458\ \mathrm{m\ s^{-1}}$$

The effect of this definition is that the metre is the length of the path travelled by light in a vacuum during the time interval of 1 ⁄ 299 792 458 of a second.

To be explicit as to "what is a metre?" the equation needs to be rearranged to give:

$$\mathrm{m} = (299\ 792\ 458)^{-1}\ c\ \mathrm{s}$$

The same numerical value is found in the current definition but in a more descriptive manner: "*the metre is the length of the path travelled by light in vacuum during a time interval of 1/299 792 458 of a second. It follows that the speed of light in vacuum is exactly 299 792 458 metres per second*." In this definition, in use since 1983, the fixed value of a constant of nature is used as the pivotal point – without having experienced adverse effects.

The Kilogram, Unit of Mass[3]

The kilogram, 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 069X×10^{-34} when it is expressed in the unit $\mathrm{s}^{-1}\ \mathrm{m}^2\ \mathrm{kg}$, which is equal to J s.

Thus, we have the exact relation

$$h = 6.626\ 069\mathrm{X}\times10^{-34}\ \mathrm{J\ s} = 6.626\ 069\mathrm{X}\times10^{-34}\ \mathrm{s}^{-1}\ \mathrm{m}^2\ \mathrm{kg}$$

The effect of this definition, together with those for the second and the metre, is to open the way to a definition of the unit of mass through two of the most fundamental equations of physics, namely $E = mc^2$ and $E = h\nu$, which related energy E to mass and to frequency, which together lead to $m = h\nu/c^2$.

To be explicit as to "what is a kilogram?" the equation is rearranged to give:

$$\mathrm{kg} = (6.626\ 069\mathrm{X} \times 10^{-34})^{-1}\ h\ \mathrm{s}\ \mathrm{m}^{-2}$$

To recognise the physical concept "mass" on the right hand side of this equation may not be self-evident to many readers. The underlying general relation, mass-to-frequency $m{\sim}\nu$, can be understood as an energy balance of matter and radiation. In this way one can show that to carry the energy equivalent to 1 kg a photon must have the frequency $\nu_{\mathrm{kg}} = 1.35\times10^{50}$ Hz, a number which is outside normal imagination. Even when splitting up the energy equivalent and distributing it over a number of photons of lower frequency, thus higher energy, this does not provide a manageable perspective; the equivalent of the kilogram being ca. 10^{32} photons of hard x-ray radiation (1 Å wavelength). This definition combines physical aspects that are usually not seen together and requires knowledge of, and confidence in, the interpretation of quantum physical phenomena.

However, the definition of a unit and its realisation ("*mise on pratique*") are two aspects that have to be distinguished. Even though the relation to frequency is stressed by the definition, at present the most promising approach to reach the necessary precision (target uncertainty) is by use of the "watt balance"[15d], a balancing experiment in which the gravitational force acting on an object is counteracted by electromagnetic induction. For this experiment a coil is suspended in a constant magnetic field. To characterize the inductive interaction between the coil and the magnetic field, the coil is moved with a constant velocity (v) and the induced voltage (U) is measured. In another step an electric current I is applied to the coil inducing an electromagnetic force of that strength that balances the gravitational force (weight) acting on a load. This load serves to realize the (New) SI unit "kilogram". Its mass, m, follows from:

$$m = UI/gv$$

where g denotes the gravitational constant which is already known with an adequate precision. Advantageously, U and I depend counter-currently on the magnetic field flux density and the coil wire length so that these parameters cancel out. The values of U and I can be measured with sufficient precision when exploiting the macroscopic quantum phenomena Josephson effect and quantum Hall effect whereby the Planck constant h comes into play. Considerable experimental progress has been achieved recently, however, to establish a world-wide net of such devices making the unit kg unrestrictedly available everywhere, a fundamental ideal of the Metre Convention, remains a future challenge.

An alternative route to realization of the kilogram has been explored in the “Avogadro Project”[15c]. It is establishing the ratio of the kilogram to the mass of an atom using an isotopically-pure single-crystal silicon sphere whose volume is measured by interferometry and whose lattice constant was determined by x-ray diffraction[34].

The Mole, Unit of Amount of Substance[3]

> The mole, 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, N_A, to be equal to exactly 6.022 141X×10^{23} when it is expressed in the unit mol^{-1}.
>
> Thus, we have an exact relation:
>
> $$N_A = 6.022\ 141X \times 10^{23}\ \text{mol}^{-1}$$
>
> The effect of this definition is that the mole is the amount of substance of a system that contains 6.022 141X×10^{23} specified elementary entities.

To be explicit as to “what is a mole?” one will deduce that it is the amount of substance made up by the specified number of elementary entities. This description leaves two questions open: what physical property is denoted by "amount" and what precisely is meant by calling the number "exact"? The ambiguity of "amount" has proved to be a permanent source of confusion and criticism up to the conjecture of circular definition[24]. It may be hoped that IUPAC's appeal to replace the term "amount of substance"[17] will not only lead to a more instructive term but also to the clarification of the underlying concept.

Concerning the number itself there is not much change as the present implicit quantification "as many elementary entities as there are atoms in 0.012 kilogram of carbon 12" is replaced by an explicit number which will be chosen to match the best estimate of "as many" at the time when the New SI is inaugurated. However the exponential (scientific) notation obscures the fact that the mole is related to entities, and therefore the numerical value of N_A should be an integer number. The exponential (scientific) notation is typical for a rounded real number, while if an integer is meant, all digits should have been spelled out[29] as was done for $\Delta\upsilon(^{133}\text{Cs})_{\text{hfs}}$ and c above and even though here 24 digits are necessary. Not doing so yields additional support to the long lasting suspicion that the chemist's understanding of macroscopic processes as a multitude of identical interactions and reactions between stoichiometrically small numbers of molecules and atoms was not and is not the focus of the SI but rather the statistical handling of ensembles (such as thermodynamic ones) and their emergent properties.

Discussion: the Pros and Cons

General

A change as fundamental as changing the definitions of base units to be used in all sections of science and engineering and in everyday living would not expect to be introduced without a degree of active and at times polarized discussion even allowing for the assurance that the new definitions will not lead to any discontinuity in the values of the units as the values chosen for the constants are as close to the existing SI units as modern means of measurement make possible[35].

Many of the arguments concerning shortcomings of the SI as a "system", its logic and consistency, raised by those critical of the New SI system are the same as those made in the debates that followed after the introduction of the mole into the SI system in 1971[36-41]. The problems arose from a lack of a clear understanding of the human and abstract concept of “number” and the confusion between the use of “unit” and “reference” in the definition of “quantity” as expressed as the magnitude of the product of a number and a unit, as recently clearly explained, in detail, by Feller[27].

The primary benefit of the re-definition of the SI units is for basic physics in general and the electromagnetic community in particular. The advantage of the ampere redefinition on the basis of the elementary charge is evident due to its clarity, simplicity and the fact that it is intuitively understandable. The kilogram goes in just the opposite direction however as it enmeshes the Planck constant in the system of units which is essential in disciplines where quantum effects are exploited. Those disciplines such as chemistry and commodity traders who have to pay for it by losing the comfort and the rigor of constants must hope that it is worth the efforts the designers of the New SI to make some constants exactly "known". Unfortunately the necessary understanding of quantum physics cannot be ascribed to the general public by *diktat* nor can existing doubts in the consistency of the New SI construct be easily switched off.

While the present system, in spite of the drift of 50 µg per 100 years of the IPK, has served analytical chemistry well and even more so commerce, trade and everyday life it is near the edge of the scientific understanding of many of our contemporaries. That an improvement is necessary at some science frontiers cannot be denied, however the enforcement of a system tailored for their needs alone must be expected to disturb those for whom the changes will have little practical effect apart from the feeling of a lack of understanding of the origin of the units they use.

The future system is based on the belief that the seven constants chosen as the basis of the New SI are truly constants over space and time in the universe. Attention has recently been drawn to the validity of this assumption[32] following the questions raised by Barrow and Hill[42] in their discussion of the results from experiments on the isotopic composition of meteorites and the adsorption of quasar radiation from deep space, the data seem to indicate that the fine structure constant α might increase with time. Thus h would not be a constant, as it depends on α. Recent data on the special variation of the fine structure constant provides evidence that it increases with cosmological distance from the earth[43]. In a detailed error analysis it was not possible to identify a single systematic effect that could emulate the observed variation in α. Thus it seems prudent to qualify the degree of constancy in Planck's constant, h, in the new SI as "*being constant in terrestrial space and in the current era time frame*". This primarily concerns the definition of the kilogram, however, the lack of true constancy in the value of α also affects the definition of the second and consequently that of the metre and the ampere. Considering this suspicion about the basis of the New SI the only true constants dictated by nature appear to be the speed of light, c, the electron charge, e, and Boltzmann's k.

In addition to the small variation in α, the general question arises as to how safe is the belief that the other constants are truly invariant, that our present models of the world are adequate and our recent measurement results reliable without any systematic error. There is also the challenge that further improved measurement capabilities may exceed the scope of the planned definitions.

There is a degree of circularity in the New SI system, for instance as the statement that the units are listed in order so that no definition involves one of the other units later in the list is open to question in that the definition of the second refers to "*the caesium 133 atom at rest and at zero thermodynamic temperature*", i.e. 0 K, prior to the New SI definition of K. Further examples are given by Feller[27(a)].

Problems also arise in understanding the New SI units due to the format chosen in which to state the definitions for the units. The definitions for all the New SI units are being given in an "explicit-constant format" rather than the more familiar "explicit-unit format" meaning that the value of some constants are defined, i.e. their values are set – in case measurement advancement proves any deviation from what we know nowadays, it will not be the numerical value of the particular constant that will be changed (as has been done so far) but the dependant units. It is feared that with fixed constants and units dependant on them our present understanding is immobilized, because observation of changes or unexpected differences, the driving force of advancement, will be obscured[25]. The explicit-constant definitions and their implications are so far from normal understanding as to drive a wedge between science and society at large[44].

For example, in the definition of the metre difficulties in comprehension arise, because it does not aid rapid comprehension of 'what is a metre?' to answer that "*The advantage of an explicit-constant format definition is that it emphasises the reference constant used in the definition, which in this case is the speed of light, and which actually defines the unit metre per second rather than the metre. It also avoids suggesting that the definition of the metre is realized by measuring the speed of light, which is not the case. The definition of a unit has to be distinguished from its realization, because experiments to realize a definition may change as experimental techniques develop, and new experiments may be devised*"[23(b)]. Furthermore, the modes of realization of the new units are not currently available to read alongside the revised Chapter 2 for the new SI brochure. To ensure transparency it is essential that the experimental means to realise each unit be made quickly and readily available to all potential users of the new SI by reference to material in the open scientific literature or in a new version of Appendix 2 "Practical realization of some important units"[1] preferably written for the scientifically-literate but non-expert in advanced metrology.

In the present SI system the units are defined, their values are exact without any “measurement uncertainty”. Consequently their basis – such as the IPK for the kilogram – is also a definition. So far the constants now selected as the basis of the New SI are measured and thus have associated measurement uncertainty. In the future their “best estimate” will be fixed and rigidly coupled to the related unit so that the value of the constant is "known" without uncertainty. Of course the uncertainty cannot be abolished by decree, but is crossed over to the previous reference phenomenon, that has in future to be measured. This effect is documented in Table 1 which has been adapted from reference 13b.

Table 1 The Effect of Changing from the Current SI to the New SI on the Relative Standard Uncertainties of the Constants used to Define the Kilogram, Ampere, Kelvin and Mole

Unit	Constant used to Define the Unit	Symbol	Relative Standard Uncertainty	
			Current SI	New SI
kg	Mass of the IPK Planck Constant	m(IPK) h	0 4.4×10^{-8}	4.4×10^{-8} 0
A	Magnetic Constant Elementary Charge	μ_0 e	0 2.2×10^{-8}	320×10^{-8} 0
K	Temperature of TPW[a] Boltzmann Constant	T_{TPW} k	0 91×10^{-8}	91×10^{-8} 0
mol	Molar Mass of ^{12}C Avogadro Constant	$M(^{12}\mathrm{C})$ N_A	0 4.4×10^{-8}	0.070×10^{-8} 0

[a] TPW – triple point of water

Specifics

The Kilogram

Aside from the explicit-constant definition, stretching the anchor (traceability) chain all through relativity theory and equivalence of mass and energy to define the kilogram may be an intellectual delight and possibly a need for a specialized community. However it leaves out many scientists and completely forgets the man-in-the-street to whom, from time to time, the money spent on science must be justified.

There is an attractive alternative to defining the kilogram: namely by relating the kilogram to the mass of an atom, such as ^{12}C, which has to date been considered as a constant of nature and is – particularly in the form of the unit dalton (Da) – closer to the hearts and to the work of the chemists and generally easier to understand and to teach[31,45]. It would also prevent problems concerning the Da/kg scale.

Regarding the precision of the kilogram, the two approaches do not make much difference, as the ratio $h/m(^{12}\mathrm{C})$ is known at a relative uncertainty of 3.2×10^{-10}. The preference for the less straightforward definition on the basis of the mass-to-energy equivalence brings h into the system and thus constants such as the Klitzing constant related to the Quantum Hall effect, what admittedly must be considered as a cornerstone in an explicit-constant system. All the more it is not only desirable but just necessary to have in Appendix 2 to the New SI Brochure not only an explanation of the actual realisation of the units but also an outline of how they are scaled down to the macroscopic needs of everyday life.

In practice, despite the difficulties of comprehending the definition of the new kilogram, its relation to h and its realisation using the watt balance[15(c)] little will change in day to day practical chemistry, due to fitting old and new at the moment of approval and the use of international prototypes of the new kilogram which for all practical purposes will be equal in mass to the old Pt/Ir standard, IPK[15(f)]. For the many analytical experiments where the result is expressed as mass fraction the mass value of the new international kilogram does not matter as the ratio of the recorded analyte (or weighing form) mass to the total mass of material cancels out, provided that the ratio of the weights within the set, or the readout values have been determined in a prior calibration.

The New Mole

The present definition of the mole refers to "*as many elementary entities as there are atoms in 0.012 kilogram of carbon 12*"[1] and thus is based on the pre-existing choice to set the relative atomic weight (mass) of the isotope carbon-12 ($A_r(^{12}C)$) to 12 exactly with zero uncertainty:

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

where M_u is referred to as the molar mass constant. The current definition adopts a value of exactly 10^{-3} kg mol^{-1}. The factor of 10^{-3} arises because of the choice of a “gram-mole” rather than a “kilogram-mole”. Retention of the carbon-12 scale is essential for the continued validity of the extensive collections of high accuracy mass spectra.

If the mole is re-defined on the basis of a fixed number of entities, then the mass of a mole of ^{12}C is given by

$$M(^{12}\mathrm{C}) = N_\mathrm{A}\, m(^{12}\mathrm{C})$$

The mass of a carbon atom $m(^{12}C)$ will become an experimentally determined quantity, then $M(^{12}C)$ will become an experimentally determined quantity. Atomic weights will no longer be constants of nature[22]. The values of the relative atomic masses remain as before provided IUPAC use carbon-12 as the scale reference. Therefore M_u must also become an experimentally determined quantity with an estimated relative uncertainty[14] of 1.4×10^{-9}. This is so small as not to have any significance in practical work.

The Mole – Old and New

Ever since the first definition of the mole by SI in 1971 it has been a subject of discussion and abundant studies into the teaching-learning of the mole concept[36-41]. Much of the discussion revolved round the meanings placed on the term “gram-atom” and the introduction of dimensional analysis (quantity calculus) to chemistry. The definition of the mole in the New SI system has not solved the previous problems and the debate continues with the additional problem that many chemists do not consider the Avogadro constant to be one of the fundamental constants of nature[24,27,29,30,31,33,46,47] rather, that it is a man-made construct.

The New SI will inherit the question as to what the mole actually is. The SI definition says it is the unit of amount of substance and outlines further[3]: "*The quantity used by chemists to specify the amount of chemical elements or compounds is now called "amount of substance". Amount of substance, symbol n, is defined to be proportional to the number of specified elementary entities N in a sample, the proportionality constant being a universal constant which is the same for all entities*"[3].

Considering the units mentioned before, the quantity they scale – time, length, mass – is intuitively understood and physically clear. However "*amount of substance*" could be just the number of entities or it could be another extensive quantity as are e.g. volume, mass or Gibbs energy. In any case it is proportional to "number" while the Avogadro constant scales it with a "package size" called mole. Surely 2 boxes of 12 eggs each bring 24 eggs, however how many indivisible entities "eggs" are in 2.1 boxes? Strictly speaking, only a minority of (real) numbers of moles corresponds to an integer number of entities, most of the continuum of real numbers does not. The size of the number (10^{23}) obscures and approximates the "discontinuity" of substance well, still the current "mole" seems to be associated to a different perception of reality, and the algebra of integers is different from the algebra of real numbers[29].

It is noteworthy that the multi-digit number of entities to be stated in the New SI makes it evident that an attomole (10^{-18} mol) – an amount of substance not nowadays outside measurement capabilities – cannot exist in strict compliance with the definition of the unit as it should comprise a 0.1X fraction of an entity.

As observed by IUPAC, the mole is often thought of by chemists as an Avogadro **number** of entities[17], then the quantity currently called "amount of substance" is just a number of entities, the mole being a convenient scaling factor for relating atomic scale entities (in which chemical stoichiometry is expressed) and macroscopic quantities (as used in bench level chemical experiments)[31,45].

Once the significance of the "new mole" is understood by chemists trained on the old SI system it will be appreciated that the numbers used in stoichiometric calculations, analytical factors and the mass ascribed to materials weighed out will be virtually unaffected. Thus they can proceed more or less as before, even if not convinced by the case for change. However, the serious question that remains is how to teach the new generation the New SI mole without involving much of the prior historical and complex development of the concept of the "mole"?

Conclusion

One could have hoped that the years of approaching the New SI would also have been used to rectify some of the shortcomings of the system's logical foundation as described e.g. by Feller[27] – so far there is no indication that such problems are being tackled. The structural novelty of the New SI is based on the strong belief in the invariance of some physical constants so that the possibility to check and monitor their values by direct measurement using units fixed elsewhere, is sacrificed – which as mentioned above is causing quite some concern. As to the individual units there is the plausible update of the ampere due to the complex construction of the kilogram in order to employ the Planck constant. Essential from the practical point of view, is the fact that the system of the seven (base) units we are used to using will continue.

So far the “man-in-the-street”, the consumer and producer of everyday products as well as the analytical or clinical chemist lives comfortably with the present SI. The IPK appears something of an historic relic, however we have been well served with the unit and its multiples and submultiples that correspond to our tasks. The New SI is tailored to the needs of the electromagnetic community and one cannot but hope this will make their work more efficient and foster great advances. Even the new superstructure on top of our system may appear fragile to the sceptic, the distance from the relative standard uncertainties in the order of 10^{-8} or better to the common levels in analytics is comfortable enough to minimize the effect of changes if such corrections should become necessary.

Originally there was the intention to make the SI easy to understand:

> *"since 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."*[10]

Full discussion of all aspects of the new SI and necessary teaching texts explaining the consequences of "explicit-constant" definitions or the Planck-Einstein kilogram are yet to appear.

It would be an advantage if at least some of the basic shortcoming of the system as such could be dealt with; in any case the educational challenge of the New SI remains.

What is the Chemist's Mole?

Life in the globalized world of science, engineering and commerce needs an unambiguous measuring system[48]. This is emphasised by fatal consequences of interpreting numbers with different units for example by the loss of the NASA Mars Climate Orbiter in 1999[49]. The sustained opposition against the SI definition of the “mole” seems to indicate that under the term “mole” two different concepts are practiced: the one described in the SI and another one being a number of entities. This will have caused the CIPM "Consultative Committee for Amount of Substance: Metrology in Chemistry" (CCQM) to request "*that, prior to the change, a more widespread understanding of the concepts and their acceptance within the chemical community must be achieved*" and its recommendation regarding the redefinition of the mole and kilogram to give *"full consideration...to the interest of the chemical measurement community*"[50].

If the continuous SI unit “mole” is necessary in certain disciplines while the pure scaling factor would serve the needs in other fields, it might be reasonable to legitimise the scaling factor in a logically and legally alternative e.g. for "use with the SI"[26] rather than enforcing or tolerating an improper use.

It is suggested that the national chemical societies and their association EuCheMS should clarify the needs and practice of their members, both in the laboratory and in education, and in case voice concerns about the "chemical" unit in the New SI.

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