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LETTER TO THE EDITOR

On the proposed redefinition of the mole

W T Chyla

Applied Science Enterprise, PO Box 22, 00-975 Warszawa 12, Poland

E-mail: chylawt@wp.pl

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Abstract
This letter calls for reconsidering the new definition of the mole, which has been proposed in the draft chapter 2 for the *SI Brochure*, posted on the BIPM website. It is argued that the list of particles should be deleted from the new definition of the mole. The necessary elements of the definition are summarized and another wording is suggested. Proposals to rename 'amount of substance' are briefly discussed.

1. Introduction

In October 2011, the 24th General Conference on Weights and Measures adopted Resolution 1, which comprehensively addressed redefinition of the SI base units [1]. The Resolution outlines principles for new definitions of the kilogram, the kelvin, the ampere and the mole, suggests rephrasing of the other three base units of the SI (the second, the metre and the candela) and calls for preparing new *mises en pratique* for the new definitions.

Since the inception of the New SI program, most research and discussions have focused on the redefinition of the kilogram, whereas redefinition of the mole has attracted less attention. In this letter, I look into the proposed new definition of the mole and conclude that it might benefit from a wider discussion. In the next two sections, I analyse the structure and wording of the new definition and conclude that it needs rephrasing. Then, I enumerate the necessary elements in the definition of the mole and suggest one possible formulation that resolves the identified problems. Next, I briefly discuss proposals for renaming the quantity 'amount of substance'. A few general remarks on the structure of definitions of base units in the New SI conclude this letter.

2. The list of particles should be deleted from the new definition of the mole

The SI unit of amount of substance is currently defined as follows [2]: '*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'. 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 proposed new definition of the mole, posted on the BIPM website [3], states that '*The mole, mol, is the 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 equal to exactly* $6.022\,14X \times 10^{23}$ *when it is expressed in the unit* mol^{-1}.'

The list of particles ('elementary entities') in the recently proposed definition of the mole is copied from the 1971 definition; the list should be deleted for the following reasons.

(1) It comprises particles chosen at random, e.g. electrons are mentioned explicitly, while protons occur implicitly in the 'ions' category. That raises a question about criteria for differentiating among particles, which make some of them worth mentioning explicitly.
(2) It is incomplete, both from the viewpoint of a chemist and a physicist, e.g. free radicals, nanoparticles (fullerenes) or photons are missing, both as individual entities (kinds of particles) or categories[1] of particles.
(3) The complete list of all kinds or categories of particles does not exist. The list of already known 'elementary entities' would have comprised thousands of entries and a

[1] In this letter, the term 'category' refers to a group of entities of the same chemical/physical nature (e.g. molecules, ions, leptons, etc), whereas the term 'kind' is more specific and refers to a given kind of particles within a certain category (e.g. methane in the category of molecules, deuterium cations in the category of ions, electrons in the category of leptons, etc).

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list of different categories of physical and chemical entities would have exceeded a hundred.

(4) The list of all kinds or categories of particles cannot be complete, as those are still being discovered, e.g. the Higgs boson. The definition of the mole should not be structured such that each discovery of a new particle or a new category of particles (e.g. supersymmetric partners of already known fundamental particles) would imply the necessity to update the definition.

(5) Even if a complete list of all kinds or categories of particles could be put together, the definition of the mole is not the appropriate place to establish or cite such a list.

(6) The authors of the new definition must have realized that the list of particles ('elementary entities') is incomplete, as they employed the expression '*any other particle or a specified group of such particles*' to cover all those unlisted entities. However, if one believes that the cited expression adequately accounts for the unlisted particles, he/she must admit that it covers *all* kinds and categories of particles; therefore, the listing of chosen individual entities in the definition (atoms, molecules, electrons, ions) becomes superfluous.

3. The term 'elementary entity' should be replaced with the expression 'entities of the same kind' or 'particles of the same kind'

The unit of amount of substance, the mole, can be rightfully used when particles are *of the same kind*; if a substance consists of a few kinds of chemical or physical entities (e.g. a mixture of gases, a complex solution or a multicomponent plasma), the amount of each constituent has to be quantified (expressed in moles) separately.

The present and the proposed new definition of the mole refer to particles of the same kind as (specified) 'elementary entities'. The term 'elementary' suggests that a given entity does not have an internal structure, which does not correctly reflect the concept of particles/entities 'of the same kind'. The term 'elementary' is not normally used in the context of chemical molecules, as they are complex entities built of atoms[2]. Also in physics, the term 'elementary' is used as the synonym of 'indivisible'[3].

Since the term 'elementary' carries such specific connotations, it seems appropriate to replace it with the expression 'of the same kind'. Criteria for considering particles (microscopic entities) as being 'of the same kind' cannot be specified in general, in the definition; they have to be determined *by the user of the SI*, depending on the situation: certain physical (or chemical) entities can be 'of the same kind' from one point of view or 'of different kinds' from another standpoint. Here are a few examples.

(1) Molecules that differ only in the isotopic composition (e.g. ^{35}Cl or ^{37}Cl in organochlorine compounds) are entities of the same kind for most chemists, while users of mass spectroscopy will consider them different; similarly, ^{235}U and ^{238}U are chemically equivalent, but they are different for physicists who use AVLIS to separate isotopes.

(2) Iodine scintigraphy: metabolism of the iodine isotope in its ground state ^{131}I and in the excited (nuclear) state ^{131}I* is the same, but those entities are of different kinds with respect to their ability to produce the gamma image for diagnostic (medical) purposes.

(3) There are numerous examples of chemical entities that can be considered 'of the same kind' or 'of different kinds' depending on the situation, e.g. tautomers (ring-chain or keto-enol tautomerism), enantiomers (optical isomers), molecules of different conformations (e.g. biologically active peptides), etc.

Therefore, the new definition of the mole should employ the expression 'particles of the same kind' or 'entities[4] of the same kind' instead of the term 'elementary entity'. Note that 'particles/entities of the same kind' are not necessarily identical, as exemplified above. It is up to the user of the SI to set the criteria for considering particles/entities as being of the same kind or of different kinds, depending on the physical situation or a chemical process.

4. The necessary and sufficient elements in the definition of the mole and an example of wording

Let us assume that a consensus is reached on deleting the list of particles ('elementary entities') in the definition of the mole; then the definition ought to comprise the following elements.

(1) The mole is the unit of amount of substance.

(2) The symbol of the mole is mol.

(3) The mole is the unit applicable to particles of the same kind.

(4) One mole is the Avogadro number of particles.

(5) The Avogadro number is the (dimensionless) numerical value of the Avogadro constant.

(6) The SI dimension of the Avogadro constant is mol^{-1} (which implicitly results from (4) and (5)).

(7) The exact numerical value of the Avogadro constant must be given explicitly.

[2] For historical reasons, the term 'elementary molecule' is sometimes used in the context of a single chemical element, e.g. the atom of oxygen O, or molecules O_2 and O_3.

[3] Even though particles that were once considered 'elementary' (e.g. the proton and other hadrons) turned out to be conglomerates of even 'more elementary' entities (quarks and gluons), they are still called 'elementary particles' for historical reasons; the constituent and indivisible (as of now) entities are usually referred to as 'fundamental particles'.

[4] To be more specific, one might consider adding the qualifier 'atomic' or 'microscopic'. However, the term 'atomic particles/entities' does not cover photons, neutrinos and subatomic particles (e.g. electrons, nucleons), whereas the mole should be defined in a way that fits the research domain of not only chemists but also physicists. The term 'microscopic particles/entities' (note that *atomic force microscopy* allows one to view single atoms and molecules) is more general, because it does not explicitly refer to the atomic level, but its intuitive meaning is also not sufficiently general and specific. Fortunately, both these qualifiers ('microscopic', 'atomic') can be safely omitted in the definition of the mole, because this unit is used in the context of very large numbers of particles ($\sim 10^{23}$), which implies that those entities must belong to the macromolecular, molecular, atomic, subatomic or elementary/fundamental particle realm rather than to the macroscopic domain.

No other elements or references should be included in the definition, because its wording should be as concise as possible. In this context, let me recall the late President Reagan, who used to say 'They can't hang you for what you don't say'; more sophisticated colleagues might prefer to evoke *lex parsimoniae* (Ockham's principle).

One example of wording of the definition of the mole, formulated along the lines stated above, is: '*The mole, denoted by the symbol mol, is the unit of amount of substance. One mole is the Avogadro number of entities of the same kind; the Avogadro number is the numerical value of the Avogadro constant that equals exactly* $6.022\,14X \times 10^{23}\ mol^{-1}$ *by virtue of this definition*.'

5. Should 'amount of substance' be renamed?

Some scientists consider that it would be advantageous to rename 'amount of substance' [4, 5]; they might have a point, for the following reasons.

(1) The word 'substance' is insufficiently general, because certain particles, such as electrons or photons, can hardly be called 'substance'.
(2) The word 'substance' is insufficiently specific, so it is often neglected and replaced by the name of a specific chemical entity, e.g. 'amount of methane'.
(3) Names of derived quantities are lengthy, so that numerous other names are in simultaneous use, e.g. 'amount of substance concentration' is also called 'amount concentration', 'substance concentration', 'concentration', 'molar concentration' or just 'molarity'.
(4) A one-word name for 'amount of substance' would be much more convenient in practical use and the derived quantities could have shorter and simpler names; this would harmonize with one-word names of some other SI base quantities (time, distance, mass), many classical (i.e. continuous) derived SI quantities (velocity, acceleration, momentum, force, torque, energy, kerma, etc) and 'newly designed' names for important quantities of the quantum domain (isospin, strangeness, colour, charm, bottomness, topness, flavour, hypercharge, chirality, etc).
(5) 'Amount' of a chemical compound may be expressed not only in moles but also in other units, e.g. in grams or gram-equivalents.

The only IUPAC-accepted replacement for 'amount of substance' is 'chemical amount'. However, (1) it is not a one-word term; and (2) its intuitive meaning does not cover entities that are of physical rather than chemical character (e.g. photons, electrons, neutrinos and other subatomic particles). So far, no one-word proposals (such as psammity, enplethy, ent, chemon or numerousness) have been accepted. This author likes the name 'numerousness', but if another term is to be designed I suggest that it refers explicitly to the (extremely large) number of particles of a given kind. Let me propose the name 'numberzil', which is designed by melting together two words that characterize the base quantity ('number' of particles + 'zillion') and can be easily transcribed into other languages. Renaming of 'amount of substance' is not likely in the foreseeable future, because it requires consensus of many international bodies (IUPAC, IUPAP, ISO, CIPM and CGPM). Moreover, implementation of the New SI has already turned out to be a challenging task and an attempt to add a new theme at this time might not serve the main cause.

6. Conclusion

The proposed definitions of all (seven) base units of the New SI have the same structure. There is a merit in following the same pattern in definitions of the four fundamental base units (s, m, kg and A), which correspond to four fundamental notions (the time, the distance, the mass and the electric charge). However, the other three base units (mol, K and cd) have a clearly different status: from the physical point of view, these are supplementary base units, adopted for convenience of users rather than for physical necessity [6–8]. Also the status of the Avogadro constant (a *convenient conventional measure* of a macroscopic number of microscopic entities) is entirely different from the status of fundamental physical constants, such as c, h and e, which are indispensable in physics, as they characterize relativistic phenomena, quantum phenomena and the strength of the electromagnetic coupling.

Therefore, it seems that there is no merit in forcing the definition of the mole into the structure that has been designed for the four fundamental base units of the New SI and some flexibility in phrasing of the definition of the mole is acceptable. One possible wording of the new definition is proposed in this paper and other proposals are welcome; there is sufficient time to work out the consensus before the next CGPM meeting in 2015, when the final decision on the redefinition of the SI base units is expected.

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