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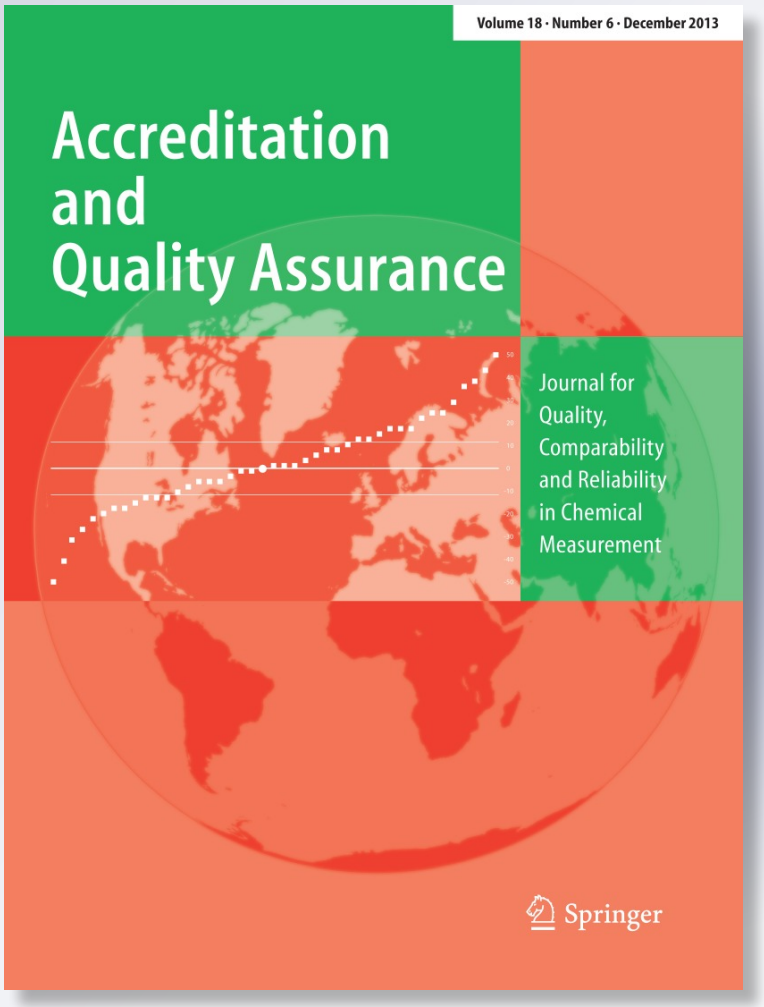

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PAUL'S COLUMN ON MIC

Second opportunity for chemists to re-think the mole

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The unit mole in the SI system of units, has been up for redefinition for some time. That task is performed through a complex committee structure.

Committee structure of the international system of units, SI (Système International)

Since several years, the seven base units, m (metre), kg (kilogram), s (second), A (ampere), K (kelvin), mol (mole), and cd (candela) of the SI, are under revision and re-definitions are being proposed by the CCU (the Consultative Committee on Units to the CIPM, the International Committee on Weights and Measures) [1]. The mechanism of such a re-definition is lengthy and not that well known, certainly not in the chemical measurement community. In essence, CCU prepares proposals to the CIPM that passes a final recommendation for decision to the CGPM (the General Conference on Weights and Measures). CGPM is convened every 4 years: 2003, 2007, 2011, then exceptionally after 3 years in 2014, then, presumably, in 2018. It decides in virtue of the powers given to it by the Diplomatic Treaty on the Metre, 'Convention du Mètre', signed in 1875.

To that effect, CCU informs (and collects opinions of) other Consultative Committees to the CIPM on units in various fields such as: Electricity and Magnetism (CCEM), Photometry and Radiometry (CCPR), Thermometry (CCT), Length (CCL), Time and Frequency (CCTF), Ionising Radiation (CCRI), Units (CCU), Mass and Related Quantities (CCM), Amount of Substance: metrology in chemistry (CCQM), Acoustics, Ultrasound, and Vibration (CCAUV).

For chemical measurement, the Consultative Committee is CCQM, which had its first session in 1996 after CIPM and BIPM had decided around 1990 [2] that there was a need for such Consultative Committee for measurements of amount of substance [3]. The opinion of CCQM is considered as very important by CCU.

Present definitions of the mole (symbol mol) and the kilogram (symbol kg)

The present definition of the mole dates back to 1971. It is given in Sect. 2.1.1.6, page 114–115 in [3]:

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.*

It follows that the molar mass of carbon 12 is exactly 12 grams per mole, $M(^{12}\mathrm{C}) = 12$ g/mol.

In 1980, the CIPM approved the report of the CCU (1980) which specified that in this definition, it is

The author is a member of the Joint Committee on Guides for Metrology (JCGM), Working Group 2 (VIM). The opinions expressed in this column do not necessarily represent the view of the Working Group nor of ACQUAL.

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understood that unbound atoms of carbon 12, at rest and in their ground state, are referred to".

The present definition of the present kilogram is given in Sect. 2.1.1.2, page 112 in [3]:

"*The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram*".

The current proposal for a re-definition of the kilogram is [1]:

"*The kilogram,* kg, *is the unit of mass; its magnitude is set by fixing the numerical value of the Planck constant to be equal to exactly* 6.626 06X $\times$ 10^{-34} *when it is expressed in the unit* s^{-1} m^2 kg, *which is equal to* J s".

And the current proposal for re-defining the mole is [1]:

"*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 $\times$ YZ $\times$ 10^{23} *when it is expressed in the unit* mol^{-1}"

where X, Y, Z are to be replaced by the best experimental values available at the moment of the re-definition.

State of the discussion of the redefinition within the International Union of Pure and Applied Chemistry (IUPAC)

The IUPAC delivered a positive advice on this proposal in 2009 at its General Assembly in Glasgow, but its ICTNS (Interdivisional Committee on Terminology, Nomenclature and Symbols) asked rather strongly for a new name to replace the confusing term 'amount of substance', covering a concept not well understood by many chemists because not well described.

As a result of CCQM invitations in 2010 noted in Sect. 7, page 9 in [4] as well as in Sect. 5, pages 7–10 in [5] for a broadest possible consultation of the chemical community at large, the Journal 'Accreditation and Quality Assurance' published a special issue with varying opinions on the re-definitions [6], some of them stressing the need for the unit one as unit for number of entities, an important concept in chemical measurement [6]. The IUPAC-CIAAW (Commission on Isotope Abundances and Atomic Weights), the very old and authoritative 'International Commission on Atomic Weights' founded as such about 1890, offered alternative proposals for the re-definitions in 2011:

"*The CIAAW*, ***noting***

1. *the request of CCQM for 'open debate …' so as to enable the preparation of an informed proposal by the CCU of a future redefinition of the mole by the CGPM,*
2. *the 2009 statement by ICTNS that the name of the ISQ base quantity 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,*
3. *the ICTNS (2009) is of the opinion that the mole is often thought of by chemists as an Avogadro number of entities,*
4. *a unanimous opinion of the WG on the mole has not yet been attained for submission to CCQM,*

and ***considering*** *that*

1. *the non-SI unit of mass, the dalton (symbol* Da*), is defined as 1/12th of the mass of a single* ^{12}C *atom,*
2. *atomic mass values for the elements are commonly expressed in daltons, not in kilograms,*
3. *all atomic weight values of the elements are also expressed in daltons,*
4. *all molecular weight values for large molecules such as proteins are also expressed in daltons,*
5. *numerous chemical measurements consist of measurement of ratios of number of entities (atoms, molecules, …),*

recommends

1. *changing the name of the quantity amount of substance to number of entities,*
2. *the following future definition of the mole:*

Mole, the unit of number of entities, symbol mol, *is a number of specified entities equal to* 6.022 14X YZ $\cdot$ 10^{23} *entities exactly.*

3. *that any decision on redefinition of the mole be deferred until full consideration is given to the interests of the chemical and isotopic measurement communities.*

and **suggests**

that together with the fixed value of the Avogadro constant, the dalton could serve to redefine the kilogram in a way that would suit the needs of the chemists:

Kilogram, the unit of mass, symbol kg, *is the mass of* 6.022 14X YZ $\cdot$ 10^{23} *atoms of* ^{12}C *in their nuclear ground state multiplied by* 1000/12,

or

Kilogram, the unit of mass, symbol kg, *is the mass of one mole of* ^{12}C *atoms in their nuclear ground state multiplied by* 1000/12".

Thus, also CIAAW specifically requested a new name to replace amount of substance, at the same time that a new definition of the mole is approved.

CIAAW informed CCQM about its position in September 2011.

Following the invitation of the CCQM for a broad consultation, the IUPAC Analytical Chemistry Division (ACD) similarly offered alternative definitions in 2012:

"Revision of the SI

As mentioned by the President, the Analytical Division has prepared its position on the proposals for revising the definitions of kilogram and mole. Supporting the stance of the CIAAW following the Antwerp Division Committee meeting [2012], the following recommendations were agreed.

In particular, we support a definition of the Avogadro ***number*** *that recognises it as a scaling factor of individual entities.*

The mole

The ACD ***recommends*** *the following future definition of the mole:*

The mole, symbol mol*, is a number of entities equal to* 6.022 14X YZ $\times$ 10^{23} *entities exactly*

Note 1: The entities must be specified

Note 2: The proposed definition does not require an associated quantity other than 1*. However, to maintain continuity with the present ISQ, the present quantity amount of substance is renamed chemical amount, and the mole be also recognised as the unit of chemical amount.*

Note 3: The International Vocabulary of Metrology (VIM) notes (1.4, Note 3) Number of entities can be regarded as a base quantity in any system of quantities.

The ACD requests that any decision on redefinition of the mole be deferred until full consideration is given to the interests of the chemical and isotopic measurement communities.

Unit of mass

If the unit of mass is no longer to be tied to the mass of an object (the International Prototype of the kilogram), the ACD proposes that the unit of mass be the gram, symbol g.

Together with the fixed value of the Avogadro number, the dalton could serve to redefine the gram. The ACD recommends the following future definition of the gram:

The gram, unit of mass, symbol g*, is one-twelfth* (1/12) *of the mass of* 6.022 14X YZ $\times$ 10^{23} *atoms of* ^{12}C *in their nuclear ground state".*

ACD released its position in its internal newsletter Teamwork in July 2013 [7]. Thus, also ACD requests that any redefinition of the mole be deferred until full consideration is given to the interests of the chemical and isotopic measurement communities.

The 1971 definition of the mole gave rise to different interpretations from its inception and continues to do so because the definition has not generated a generally accepted common understanding of the mole. In addition, the then conceived concept amount of substance was not helpful either: even the CCU asked IUPAC in its 2009 General Assembly in Glasgow, to provide a better name for the concept amount of substance, which means asking for a better term to describe that concept. That request is unanswered until this very day.

The concept number of entities is mentioned in the VIM as being a base quantity in any system of quantities (i.e. in the ISQ, the International System of Quantities on which the SI is based) as described in entry 1.6 in [8]. Similarly, its associated unit one (symbol 1) is a base unit in any system of units (i.e. also in other systems of units than the SI). See Sects. 1.4 Note 3 and 1.10 Note 3 in [8]. It is noteworthy that, in the present definition, the number of entities contained in 1 mol was equal to the number of ^{12}C atoms making up 12 g of ^{12}C, thus relating the mole to the kilogram. Remarkably, that link to the kilogram is now being cut in the proposal for re-definition.

As one can see, the re-definitions proposed by CCU [1] for mole and kilogram are rather abstract (they are based on quantum-physical considerations). In particular, they are based on the (impressively looking) relationship of the units associated with electromagnetic quantities. However, the new definitions are seen by many teachers and educators in chemistry as unnecessarily difficult to teach to a wide school public ranging from high and middle schools to graduate university classes.

Probably the most basic criticism one can have on the proposed re-definitions is the fact that the concept of constancy of units is abandoned: a unit is not anymore based on a defined value of the quantity with which it is associated. That violates a very basic and simple, traditional rule which deserves to be respected.

As a result of the reigning confusion in the chemical community, the IUPAC has now decided (in its August 2013 General Assembly in Istanbul) to start a formal interdivisional consultation amongst its divisions and standing committees, on the re-definition of the mole (and -maybe-) on the kilogram, another unit which is much used by chemists. Other chemical communities such as EURACHEM, CITAC, ISO-REMCO, EuCheMS, and ILAC should join and enrich the discussions.

A number of comments from the chemical community (and others as well) were already published in this Journal in March 2011 [6], and various comments on the proposals for re-definition are assembled in a website for discussion [9].

Thus, time has come for chemists to grasp the second, present opportunity to re-think the mole in the next 20 months.

As usual, any comment, question, or amendment is welcome, preferably as a contribution to the Discussion Forum of this Journal.

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