Accred Qual Assur (2014) 19:323–325
DOI 10.1007/s00769-014-1068-1

PAUL'S COLUMN ON MIC

CCQM owes chemists a description of the concept 'amount of substance'

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Published online: 15 July 2014

CCQM, the 'Consultative Committee on amount of substance—metrology in chemistry' to the International Committee for Weights and Measures (CIPM), is being renamed 'CC on amount of substance—metrology in chemistry and biology'.

This seems to be an excellent occasion to review the status of the understanding of the concept 'amount of substance' in the chemical community at large.

It is broadly admitted that the concept (and term) 'amount of substance' has been a source of confusion ever since it was used in the International System of Units (SI) in 1971 by the General Conference on Weights and Measures (CGPM) as the base quantity for the definition of the unit mole [1]. Thus, the International Organization for Standardization (ISO) through its Technical Committee 12, responsible for quantities, added it as such to the International System of Quantities, ISQ [2]. It was also included in the 2nd and 3rd edition of the International Vocabulary of Metrology [3, 4].

The term mole had been in existence for a very long time (almost a 100 years), albeit subject to various interpretations. However, there is a long-standing problem. A unit—of necessity—requires a quantity of which it is the unit: the kilogram is the unit of the quantity 'mass', the second is the unit of the quantity 'time', the metre is the unit of the quantity 'length', etc. The absence of a clearly understood and accepted description in the chemical community of the quantity 'amount of substance' having the unit mole, especially in the analytical community, was—and still is—a problem.

That is not good.

Sometimes, 'amount of substance' is simply described as 'the quantity of which the mole is the unit' [5, 6], a description from which we do not really learn very much. Neither is the text in a well-known textbook helpful wherein it is stated that 'The mole is an SI base unit … The physical quantity to which it refers is called the 'amount of substance', *n.* However, practicing chemists commonly prefer to talk about the number of moles. Take the advice of your instructor on whether to use or not the official term' [7]. A very worthwhile attempt was already made in 1990s to replace the term 'amount of substance' by 'numerosity' [8], a term for indeed a property of matter (see definition of 'quantity' in [3, 4]) that stresses the fact that matter is discontinuous in structure and consists of discrete entities. It was not disapproved in the literature (on the contrary) nor considered and replied to in the 'New SI' [9]. Rather 'amount of substance' was kept, stressing a continuous character as property of matter, a property that was disqualified by modern science since more than a hundred years. Also, the 'Reproposition' [10] of the suggestion underwent the same fate rather than be examined seriously.

Hence, let us attempt to understand—or at least attempt to clarify some problems—with the SI quantity 'amount of substance'.

Around 1990s, the need for 'traceability of chemical measurement results to the SI' started to take off in the literature because there was a rising need to compare measurement results across borders in trade, in commerce, in food and feed measurements, in environmental and clinical measurements, in international and intercontinental interlaboratory comparisons, to name just a few. Also,

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around 1985–1990, a change of paradigm occurred in the thinking of CIPM and its International Bureau for Weights and Measures—BIPM. Apparently, it came to mind that chemical measurements in general i.e. other than those developed for use in physical chemistry, for instance in analytical chemistry, should be considered for inclusion in the SI.

To learn more about the needed concepts, a workshop on 'Comparability and Traceability in Measurements of Amount of Substance' took place in the Central Bureau for Nuclear Measurements, CBNM (renamed Institute for Reference Materials and Measurements—IRMM in 1993). It was patronized by the 1990-born Eurachem (a European Association of Analytical Chemistry Laboratories) and intended to clarify the basic concepts involved in chemical (also called analytical) measurement.

So it was decided to set up a 'Consultative Committee on amount of substance' in 1993. It met for the first time at BIPM in April 1995.

The Terms of Reference of this Committee were (and still are):

1. to advise the CIPM in matters relating to the accuracy of quantitative [*Note of this author: not 'qualitative'*] measurements and traceability to the SI
2. to coordinate the activities of national metrology laboratories in establishing this traceability at the highest level
3. to stimulate the understanding of the concept of uncertainty and the assignment of uncertainty statements in chemical measurements, thereby encouraging the establishment of traceability taking into account other initiatives at regional and international levels
4. to keep under review the question of whether or not there is a need for a programme of work at the BIPM to support this activity

There is nothing about 'amount of substance' although one would expect some description of the concept, and some elaboration of its basic characteristics in view of the fact that it was—and still is—of key importance in the title, the task of CCQM and … its scientific-metrological authority. Instead, only the concepts 'traceability' and 'measurement uncertainty' are mentioned.

The UK Government Chemist, present in the 1st CCQM session even expressed 'concern that the work of CCQM at the highest metrological level may not be seen by the chemical community to be relevant to work at the field level'.

This statement was almost a prophecy: at the 20th CCQM meeting in April 2014, Brynn Hibbert, currently President of the Analytical Chemistry Division of IUPAC, reported that 'a review of 18 first-year university general chemistry textbooks published 1989–2014 with 14 publishers from Europe and the USA (writing in English), reveals that the concept 'amount of substance' is

- mentioned in the index in 3 cases out of 18 only, and
- referred to in the text correctly in 4 cases out of 18 only'.

He also observed 'that a correct SI definition of the mole is given in zero cases out of 18' and—with respect to 'amount of substance'—asks the question 'do we need it ?' (B Hibbert, personal communication). This is not a big improvement since ''Strömdahl et al. carried out an interesting study on the concept of mole among educators in 1994 and found that only 11 % identified the mole as the unit of 'amount of substance'' (quoted in [11]).

The present revision of the SI offers an excellent opportunity for CCQM to provide its own simple clarification of the concept 'amount of substance' and improve its understanding and usefulness by a clear and handsome description that meets the chemist's needs. Whilst some chemists tend to shorten the term to 'amount' and other, e.g. in the clinical measurement community, prefer to stay with 'substance' for the concept, the ongoing definition of the associated unit mole should be reconsidered in the light of a better described base quantity 'amount of substance'.

So, from no description, a base concept in the ISQ in 1971, until now, not much seems to have happened. There were appeals to rethink the concept of the base unit 'mole' and its base quantity 'amount of substance' [12, 13] as well as a number of critical papers on the concept 'amount of substance' and the 'mole', a number of them referred to in the list of references hereafter.

The problem of not understanding 'amount of substance' was exacerbated in 2009 when the IUPAC asked CCQM for an alternative/better name for 'amount of substance' [14]. CCQM still owes a reply to that question. A critical remark on the name was even formulated by the CCU President [15]. In the meantime, a very informative set of treatments of the problems related to the concept 'amount of substance' was released on a website [16]. The fact that the CCU proposal for redefinition of the mole is based on the widely understood Avogadro *constant*, N_A, with the incomprehensible dimension of *reciprocal* amount of substance and is also a source of much confusion [17, 18]. In 1996, M McGlashan already wrote about the concept 'amount of substance': 'Do we really need amount of substance? No, we could perfectly manage without the introduction of amount of substance'. And: 'If any change was needed …, then that of abandoning amount of substance altogether would be much less unattractive. Though widely used by chemists, the physical quantity called amount of substance and its SI unit called the mole are not necessary in science' (1996, personal communication). However, the concept was maintained.

One of two truly seminal papers for all metrologists looking forward to the future of the SI (and worth priority reading) summarizes the present situation as follows: 'the concept and definition of the amount of substance and mole are problematic' and 'The SI amount of substance is a redundant quantity'. It concludes: 'rename 'amount of substance' and clarify the status of the mole'. This quote is no less than part of a call 'to make [the SI] a rational, elegant system that reflects the rationality and elegance of science' [19, 20].

How can a revision of the unit mole be conceived when there is such a variety of well-argued scientific opinions in the (chemical) measurement community about 'the quantity for which the mole is supposed to be the unit'? Can any kind of revision of the SI on this point yield a useful result as a matter of principle?

What is 'amount of substance'? Do we need it? The answers to these questions should come from CCQM.

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

References

1. 14th International Conference on Weights and Measures (1971) BIPM, Paris-Sèvres. http://www.bipm.org/en/CGPM/db/14/3/
2. ISO 80000-8 (2007) Quantities and units—part 8. International Organization for Standardization, ISO, Geneva
3. BIPM, IEC, IFCC, IUPAC, IUPAP, ISO, OIML (1993) The international vocabulary of basic and general terms in metrology (VIM) (2nd edn.) entry 1.12. International Organization for Standardization, ISO: Geneva
4. BIPM, IEC, IFCC, ILAC, IUPAC, IUPAP, ISO, OIML (2012) The international vocabulary of metrology—basic and general concepts and associated terms (VIM) (3rd edn) JCGM 200, entry 1.16. http://www.bipm.org/vim
5. Baranski A (2011) The atomic mass unit, the Avogadro constant, and the mole: a way to understanding. J Chem Educ 89:97–102
6. Emerson WH (2014) The SI's base quantities and units. http://www.MetrologyBytes.net/opEds2014.php
7. Atkins P, Jones L (2000) Chemical principles, the quest for insight. Freeman & Co, New York, pp F43–F45
8. Rocha-Filho RC (1990) A proposition for the quantity of which the mole is the unit. J Chem Educ 67:139–140
9. http://www.bipm.org/utils/common/pdf/si_brochure_draft_ch123.pdf
10. Rocha-Filho RC (2011) Reproposition of numerosity as the SI base quantity whose unit is the mole. Accred Qual Assur 16:155–159
11. Furio C et al (2002) The learning and teaching of the concepts 'amount of substance' and 'mole': a review of the literature. Chem Educ Rev Res Pract: Concepts 3:277–292
12. De Bièvre P (2013) Second opportunity for chemists to re-think the mole. Accred Qual Assur 18:537–540
13. De Bièvre P (ed) (2011) The re-definition of the mole must be of high quality. Accred Qual Assur 16:117–174
14. IUPAC (2009) Report of IUPAC/ICTNS meeting in Glasgow, see minutes 8.2.4.4. http://www.iupac.org/fileadmin/user_upload/standing/ictns/ICTNS_09other-reports.pdf and http://www.iupac.org/body/027
15. Mills I, Milton M (2009) Amount of substance and the mole. Chem Int 31:1–7. http://www.iupac.org/publications/ci/2009/3102/1_mills.html
16. http://www.MetrologyBytes.net/opEds2014.php
17. Leonard BP (2014) The mole is an Avogadro number of entities, the macroscopic unit for chemical amount. Accred Qual Assur 19:213–220. doi:10.1007/s00769-014-1047-6
18. Johansson I (2014) Constancy and circularities in the SI. http://www.MetrologyBytes.net/opEds2014.php
19. Foster M (2010) The next 50 years of the SI: a review of the opportunities for the e-science age. Metrologia 47:R41–R51
20. Cooper G, Humphry SM (2012) The ontological distinction between unities and entities. Synthese 187:393–401