IUPAC Mole Project meeting minutes

29-31 January 2015

National Research Council Canada, Ottawa

EXECUTIVE SUMMARY

With a remit to provide a critical assessment of the definitions for the quantity amount of substance and its SI unit, mole, the Task Group held its third meeting. After three-day discussions of peer-reviewed literature related to the new SI in general and the mole in particular and analysis of the replies from IUPAC National Adhering Organizations, the Task Group members concluded that the CIPM-proposed future definition of the mole would satisfy a general demand for a clearer definition of the mole. An informative paragraph was drafted for consideration by the drafting committee of the SI Brochure (9th edition) and the Task Group members present voiced their unanimous preference for "chemical amount" as the name of the quantity for which mole is the name of the SI base unit (symbol mol).

REMIT

This project aims to achieve internal IUPAC consensus on the definition of the mole. The outcome of this project will be an IUPAC Technical Report which may not change the official IUPAC position on the mole that was ratified by the IUPAC Council in 2011. Any change of the IUPAC position will need to be proposed to and ratified by the IUPAC Council.

VENUE AND DELEGATES

IUPAC Project 2013-048-1-100 Task Group held its third meeting at the National Research Council Canada in Ottawa on 29-31 January 2015. The following were present:

Task Group Members

Juergen Stohner (JS), *Zürich University of Applied Sciences (Switzerland); Chair of the Task Group, Chair of IUPAC Commission I.1, Secretary of IUPAC ICTNS, and Titular Member of IUPAC Division I*

Roberto Marquardt (RM), *University of Strasbourg (France); President of IUPAC Division I and Member of IUPAC Bureau*

Zoltan Mester (ZM), *National Research Council Canada; Secretary of IUPAC Division V*

Juris Meija (JM), *National Research Council Canada; Chair of IUPAC CIAAW and Titular Member of IUPAC ICTNS*

Marcy Towns (MT), *Purdue University (USA); Titular Member of IUPAC CCE*

Invited experts

Richard Davis (RD), *International Bureau of Weights and Measures (retired); former Executive Secretary of CCM (BIPM)*

Barry Wood (BW), *National Research Council Canada; Vice-chair of CODATA Task Group on Fundamental Constants*

Apologies

Ron Weir, *Royal Military College of Canada; Chair of IUPAC ICTNS*

Abbreviations used in this report

BIPM: International Bureau of Weights and Measures
CCE: IUPAC Committee on Chemistry Education
CCEM: CIPM Consultative Committee for Electricity and Magnetism
CCQM: CIPM Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology
CCM: CIPM Consultative Committee for Mass and Related Quantities
CCU: CIPM Consultative Committee for Units
CGPM: General Conference on Weights and Measures
CIPM: International Committee for Weights and Measures
CIAAW: IUPAC Commission on Isotopic Abundances and Atomic Weights
CODATA: The Committee on Data for Science and Technology
ICTNS: IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols
IPK: International Prototype of the Kilogram
ISQ: International System of Quantities
IUPAC: International Union of Pure and Applied Chemistry
IUPAP: International Union of Pure and Applied Physics
NAO: National Adhering Organization of IUPAC
SI: The International System of Units
VIM: International Vocabulary of Metrology

1. OPENING OF THE MEETING

Task Group Chairman JS opened the meeting at 9:40 a.m. and expressed his best wishes to Task Group member Ron Weir (Chairman of ICTNS), who could not attend. The following agenda was adopted for the meeting:

1. Opening of the meeting and adoption of the minutes of the last meeting (JS)
2. The new SI: its origins & structure (BW)

3. Discussion of the peer-reviewed literature and free discussions
4. Analysis of the replies of IUPAC NAOs
5. Distribution of tasks and closing of the meeting

The minutes of the 2014 Zurich meeting were approved and now constitute the official record of that meeting. These minutes have been deposited with the IUPAC Secretariat and are available publicly on www.iupac.org.

The Task Group discussed the outline of the Technical Report and decided to include statements regarding the perceived conflicts of interest. For example, RD (an invited expert) represents BIPM, JM represents CIAAW, and ZM represents IUPAC Analytical Chemistry Division and all of these bodies have issued public opinions on the matter of redefinition of the mole. All Task Group members asserted that they were not biased by the opinions of the Organizations they represent and that the critical evaluation of the proposed definition was carried out by analyzing the practical and pedagogical advantages and/or disadvantages. For his part, RD made the same assertion. It was also unanimously decided that RD will be a coauthor of the IUPAC Technical Report produced by this Task Group.

2. THE NEW SI: ITS ORIGINS & STRUCTURE

BW gave a talk entitled "The New SI: Its Origins & Structure". The main focus of the talk was on the fundamental constants and their role in scientific measurements and in the new SI. Although the name "SI" dates from 1960, the SI evolved from the MKS system introduced in the 1880s. As the name implies, the MKS system had three base units (m, kg, s), all independent and with the metre and kilogram defined through artifacts conserved at the BIPM. The kilogram was—and remains to this day—defined by the mass of the international prototype of the kilogram, the IPK (approximately the mass of a litre of water), the meter was defined by the length of the international prototype of the metre (approximately 10^{-7} the length of the quadrant of the Earth), and the second was defined as 1/86400 of the mean solar day as determined by astronomy. These three base units clearly did not address all measurements. For example, electrical and chemical measurements were routinely performed outside the SI. BW gave examples of measurements that span large dynamic ranges. For example, resistance measurements are performed from 10^{-27} Ω to 10^{18} Ω thus spanning 45 orders of magnitude. Likewise, length measurements are performed from the current upper-limit of the asymmetry of the electron (10^{-29} m) to the diameter of Earth orbit (10^{11} m) thus covering 40 orders of magnitude. Given that physical artifacts are almost impossible to access over these ranges, fundamental constants are

essential to realize near perfect scaling over these enormous ranges. On the question of what is a fundamental constant, BW replied that fundamental constants are the basis of how we describe all our observations. Given that chemists perform mass measurements in kilograms, and given that they commonly refer to the atomic weights, which are expressed as ratios of atomic masses, the scaling factor between atomic masses and the macroscopic mass of the SI kilogram constitutes an important constant for chemists. It is irrelevant whether "the Avogadro constant is a fundamental constant of a lesser breed" (quoted from *Chem. Intl.* 2010, **32**, p.10) as compared to the Planck constant or the speed of light. What matters in practice is that scientists find this constant useful. Similar to the Avogadro constant, the Boltzmann constant is also a scaling factor. Although neither of these constants is strictly necessary in science, they have been proven useful.

BW explained that fundamental constants are the best standards that we have, and we have known it for some time. In fact, the use of fundamental constants in the SI has a long history dating from initiatives begun in 1948. The present definition of the ampere (since 1954), for example, has the effect of fixing the numerical value of the magnetic constant (μ_0) when it is expressed in the SI unit of henry per metre (note that H/m = N/A^2). Likewise, the current definition of the metre (since 1983) has the effect of fixing the numerical value of the speed of light in vacuum when it is expressed in the SI unit of metres per second. Together, these two definitions have also the effect of fixing the numerical value of the electric constant ($\varepsilon_0 = \mu_0^{-1}c^{-2}$) when it is expressed in the SI unit of farad per metre. The ampere is the present base unit, but the farad is also uniquely defined. In this vein, the proposed "new SI" also blurs the distinction between base units and derived units by stipulating exact numerical values of several constants in order to set the magnitude of the SI base units. The set of seven defining constants is merely a judicious choice, reflecting modern science and technology. The concept of "seven base units" has become more than ever a historical anachronism. For example, when the hyperfine splitting of caesium-133, the Planck constant, and the elementary charge are all given fixed values, the ampere becomes uniquely defined, and so are the volt and the ohm. For historical continuity we may continue to think of the ampere as a base unit but its metrological status will be no different to that of the volt or the ohm. Realizations of the units defined by constants of nature are possible using more than one method. For example, the ampere can be uniquely defined by the second and the elementary charge. One can, however, realize this definition in two ways: (1) through the Josephson effect (for electrical tension) and the quantum Hall effect (for resistance), relying on Ohm's law to obtain the current or (2) by single-electron tunneling.

Likewise, the kilogram can be defined by the Planck constant or it can be defined by the dalton and realized via watt balances or x-ray crystal density measurements in both cases. Ultimately, all decisions regarding the units are agreed by consensus and practical considerations play an important role.

3. DISCUSSION OF THE PEER-REVIEWED LITERATURE

The Task Group had reviewed over seventy published articles that have appeared in the peer-reviewed literature from 1961 to 2015 dealing with the definition of the mole. These discussions took more than two days. Due to the free nature of most discussions, it was not feasible to record all issues raised during the meeting. However, several main points merit a note (in no particular order). BW commented that the best measurements are those which involve counting. Consequently, the proposed definition of the mole would reflect this reasoning even though there is no apparent benefice from this definition.

A common thread throughout the literature was the confusion between the definition of a unit and the realization of a unit. This is perhaps most evident in the critiques of the proposed definition of the kilogram in terms of a fixed numerical value of the Planck constant. To some this suggests that the definition is now tied to the watt balance. However, the fixed-*h* definition of the kilogram does not prevent one realizing the kilogram by means of the x-ray crystal density method. The purpose of the formal unit definition is not to provide a description accessible to secondary school teachers or students. Rather, it serves to underpin the quality of the best measurements in the world. In regards to the often raised comment that the proposed definition "leaves out many scientists and completely forgets the man-in-the-street" (quoted from *J. Assoc. Public Analysts* 2013, **41**, 28–44), the Task Group noted the recent publications of LEGO watt balances appropriate for interested secondary school students[1]. The critics often suggest that defining the kilogram as the mass of a certain number of atoms would be comprehensible to all. One problem, however, is that such a definition would be impossible to realize as imagined because of the time it would take to count the number of atoms contained in one kilogram. If counted at the rate of one atom per second, the time needed would be many orders of magnitude greater than the age of the universe. Consequently, one cannot estimate the number of atoms in such samples by counting them. One can do so, however, via the ratio of the mass of the sample to the mass of an individual atom by means of sophisticated experiments. This shows that one has to carefully separate the

[1] Chao, L.S. et al (2014) A LEGO watt balance: An apparatus to demonstrate the definition of mass based on the new SI, arXiv:1412.1699 [arxiv.org/abs/1412.1699]. See also a manuscript by Quinn, T. et al (2013) *Phys. Educ.* **48**, 601 [doi: 10.1088/0031-9120/48/5/601]

teaching aspects and the practical aspects of measurement science. In addition, the *mises en pratique* outlining how to realize definitions of units are not intended to be didactic. Thus the challenge remains to rephrase definitions intended to serve measurement science such that they become comprehensible for the "man-in-the-street", analogous to the way the definition of the second, realized by a caesium atomic clock, has been explained.

ZM summarized the peculiar situation of the mole in contradistinction to the kilogram or ampere. The proposed definitions of kilogram and ampere have been carefully selected in order to improve the realization of these units. On the contrary, chemists have spent considerable efforts to debate the current and proposed definition of the mole despite the fact that the realization of this measurement unit remains unaffected. JM noted that this comment mirrors the sentiments voiced by Theodore W. Richards in 1901 in regards to the debates over the choice of hydrogen or oxygen as the atomic weight unit:

> "One regrets that so much time should have been spent in discussing a matter which involves no fundamental principle, but is simply a question of form and of convenience".[2]

Many authors comment that the current definition of the mole and the quantity amount of substance lacks understanding in educational communities (teachers and students). However, MT pointed out that this lack of understanding does not prevent teachers and students from carrying out stoichiometric calculations.

Name of the quantity "amount of substance"

In the educational literature there is confusion among students, teachers, and textbook authors regarding the phrase "the amount of substance". In 2009, ICTNS adopted a motion to recommend to the IUPAC Bureau 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" [ICTNS 2009 Minutes, §8.2.4.4]. This recommendation was approved unanimously by the IUPAC Executive Committee during its 141st Meeting in December 2009. Pursuant to the above recommendation, this Task Group discussed a suitable alternative name for the "amount of substance". A discussion arose regarding many proposed names for the quantity and "chemical amount" emerged as the best choice. As some authors have reflected[3], 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, JS commented that there is a widespread misunderstanding in

[2] Richards, T.W. (1901) The Standard of Atomic Weights. *Proc. Am. Acad. Arts Sci.* **37**, 177–181
[3] Leonard, B.P. (2014) *Accred Qual Assur* **19**, 213–220 [doi: 10.1007/s00769-014-1047-6]

regards to the use of the name “amount of substance”. IUPAC Green Book (3rd edition) points out [§2.10] that “the words ‘of substance’ may be replaced by the specification of the entity”. Hence, in practice we speak of amount of oxygen and not amount-of-substance of oxygen. In that sense, “amount of substance” is a placeholder name and “chemical amount” would avoid this misunderstanding. In addition, the word “chemical” can be omitted when sufficient context permits much like the name “electrical current” is often shortened to “current” in the scientific literature.[4] For example:

> chemical amount of dioxygen is 5 mol, $n(O_2) = 5$ mol
> chemical amount of iron(III) oxide is 2 mol, $n(Fe_2O_3) = 2$ mol
> amount of dioxygen is 5 mol, $n(O_2) = 5$ mol
> amount of iron(III) oxide is 2 mol, $n(Fe_2O_3) = 2$ mol.

In fact, “chemical amount” appears as an alternative name for “amount of substance” in IUPAC Green Book since 1993.[5] This Task Group decided 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.

Definition of the quantity

Several IUPAC NAOs have expressed their dissatisfaction with the current formal definition of the quantity “amount of substance”. Although not explicitly “defined” in the IUPAC Green Book, the information given therein is used as the de facto definition of the quantity worldwide. In particular, it provides “$n = N/N_A$”. JM expressed the opinion that we should aim to provide a description of the quantity which goes beyond verbalizing the above expression. The following text was proposed by the Task Group as an honest union of opinions (with slight modifications after the meeting):

> 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 $6.022\ 140\ 86 \times 10^{23}$ elementary entities. This number of elementary entities is called the Avogadro number.[6]

[4] When chemical amount appears in the denominator of compositional kind-of-quantities, such as *m*/*n* or *V*/*n*, both IUPAC GreenBook and IUPAC SilverBook recommend the adjectival form “molar” for the name of these compositional quantities (e.g., molar mass, molar volume) despite the reluctance from ISO and despite the fact that this adjective involves the name of a unit. This is done because of the established historical tradition and lack of better alternatives.

[5] The name “chemical amount” would have appeared in the 7th edition of the SI Brochure (2006) in Section 2.1.1.6 entitled “Unit of amount of substance (mole)” but was removed during the 16th meeting of CCU at the request of Prof. Thor (16th Meeting of CCU; Minutes 4.4).

[6] We employ here the 2014 CODATA recommended values (http://physics.nist.gov/cuu/Constants/)

Chemical amount of a substance B, n_B, is proportional to the mass of a substance B, m_B, and also to the number of entities, N_B:

$$n_B = (M_B)^{-1} m_B$$
$$n_B = (N_A)^{-1} N_B$$

The proportionality constant between chemical amount and mass is the reciprocal of the molar mass, which is unique to each substance, whereas the proportionality constant between chemical amount and number of entities, the reciprocal of the Avogadro constant, N_A, is the same for all substances. 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 regarded as dimensionless (or as having the dimension 1). The Avogadro number, 6.022 140 86 x 10^{23}, is the numerical value of the Avogadro constant, N_A = 6.022 140 86 x 10^{23} mol^{-1}. The previous definition of the mole implied that the Avogadro number is the mass ratio of the kilogram to the atomic mass unit, the dalton. The historical continuity of the present definition preserves this relation to within a negligible uncertainty.

The molar mass of any atom or molecule B, M(B), may still be obtained from its relative atomic mass (atomic weight), A_r(B), from the equation

$$M(B) = A_r(B)[M(^{12}C)/12] = A_r(B)M_u$$

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

$$M(B) = N_A m_a(B) = N_A A_r(B) m_u$$

and m_u is the atomic mass constant (dalton), equal to $m_a(^{12}C)/12$. M_u and m_u are related with the Avogadro constant through the relation $M_u = N_A m_u$.

Definition of the unit

Many educational manuscripts on the mole and surveys alike emphasize that teachers teach and understand the mole as the unit of a quantity representing an Avogadro number of entities. This sentiment is also reflected by the ICTNS (2009 Minutes, §8.2.4.4) and the new definition of the mole is aligned with this view as it no longer specifies the magnitude of mole contained in a certain mass (of carbon 12) but rather the exact number (the Avogadro number) of entities contained in a mole.

Avogadro constant

Many authors argue that the Avogadro constant is not well understood. In fact, there is a widespread divergence of opinion about the nature of the Avogadro constant:

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. This Task Group takes the position of CODATA Task Group on Fundamental Constants on this matter and considers the Avogadro constant an important tool used by chemists. It is of little value to argue whether a certain concept is "fundamental" or not as any such discussions will abound with subjective opinions. Others argue that there is no need to involve the Avogadro constant in any SI definition and that one could simply define the mole in terms of two units of mass: the kilogram and the atomic unit of mass (the dalton). Leonard, for example, contends that one has to recognize the Avogadro number, which is equal to the gram-to-dalton mass ratio, and then stipulate that mole is the amount of substance which contains the Avogadro number of entities. This Task Group has followed such an approach in the previous section.

Compatibility between molar mass and atomic weight

Maintenance of compatibility between the molar masses and atomic weights is concerning to some. In short, some authors maintain that chemists enjoy the identity between the numerical values of atomic weights and molar masses. For example, the molar mass of mercury is $M(\mathrm{Hg})$ = 200.592 g/mol and the standard atomic weight of mercury is $A_r(\mathrm{Hg})$ = 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 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 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, with a difference between the two numerical values currently being in the order of one part in 10^9. Consequently, many contend that the expression relating molar mass and atomic weights, $M(\mathrm{X}) = A_r(\mathrm{X})M_u$ will lose its appeal since M_u will no longer remain to be 1 g/mol exactly. This problem can be reformulated by introducing a "correction factor":

$$M(\mathrm{X}) = (1 + \kappa)A_r(\mathrm{X})M_u$$

which allows M_u to remain 1 g/mol exactly. The Task Group dismisses the concerns in regards to the "incompatibility" between molar masses and atomic weights and has made several observations in this regard.

A discrepancy in the molar mass at the level of one part in 10^9 is not in the realm of concern for chemists. To date, the most precise chemical measurement, so to speak, is the measurement of the molar mass of a 1 kg single crystal of silicon, highly-enriched in silicon-28. This project has benefited from extraordinary financial support from the International Avogadro Consortium and, in 2014, the lowest reported expanded uncertainty of the molar mass of the enriched silicon sample reached 3 parts in 10^9.[7] Virtually all chemistry measurements perform at precision levels several orders of magnitude worse. In addition, there are only three elements whose standard atomic weights are currently with precision below one part in 10^9: sodium, fluorine, and phosphorus. Hence, the fact that the molar mass of carbon-12 will now have an uncertainty of few parts in 10^9 can have an impact on the molar masses of only a handful of substances such as F_2, P_4, 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.[8] Chemists do not work with unbound atoms and binding energy between atoms leads to the loss of mass ($\Delta m = E/c^2$). Consequently, the mass of chemical substances does not equal the atomic mass times the number of entities. The molar mass of crystalline substances is given by $M(\mathrm{X})_{\mathrm{cr}} = A_{\mathrm{r}}(\mathrm{X})M_{\mathrm{u}} - \Delta_{\mathrm{f}}H^0{}_{\mathrm{c}}(\mathrm{X})/c^2$ where $\Delta_{\mathrm{f}}H^0{}_{\mathrm{c}}(\mathrm{X})$ is the cohesive energy of the crystal.[9] For a graphite crystal, $\Delta_{\mathrm{f}}H^0{}_{\mathrm{c}}(\mathrm{C}) = 711$ kJ/mol which corresponds to a relative difference between the molar mass of bound and unbound carbon-12, $M(\mathrm{C})_{\mathrm{cr}} - M(\mathrm{C})$, of almost one part in 10^9. 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" should be avoided at all costs is unreasonable. 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 proposed definition of the mole.

4. CONSULTATION WITH IUPAC NAOs

Questionnaire: general

The letter to NAOs was sent out in June 2014 to the official representatives of IUPAC National Adhering Organizations using email addresses as they appear on iupac.org.

[7] Vocke, R.D. Jr et al (2014) Absolute silicon molar mass measurements, the Avogadro constant and the redefinition of the kilogram. *Metrologia* **51**, 361 [doi:10.1088/0026-1394/51/5/361]

[8] At the request of IUPAC, this stipulation was formally endorsed by CIPM at its 1980 meeting by specifying that "it is understood that unbound atoms of carbon 12, at rest and in their ground state, are referred to".

[9] Davis, R.S and Milton, M.J.T. (2014) The assumption of the conservation of mass and its implications for present and future definitions of the kilogram and the mole. *Metrologia* **51**, 169 [doi: 10.1088/0026-1394/51/3/169]

The announcement of this activity was published in the official IUPAC news magazine in July 2014 (*Chem. Intl.* 2014, **36**, ii, doi: 10.1515/ci.2014.36.4.ii) and in September 2014 (*Chem. Intl.* 2014, **36**, 17, doi: 10.1515/ci-2014-0517). In addition, an announcement of this consultation also appeared in August 2014 in the journal Accreditation and Quality Assurance (*Accred. Qual. Assur.* 2014, **19**, 411–412, doi: 10.1007/s00769-014-1074-3), an announcement of this action was posted on the IUPAC NAO forum of IUPAC Discussion Board (at forum.iupac.org) by the IUPAC Secretariat (10 July 2014), and RM notified the IUPAC Bureau at the 95th Meeting of the IUPAC Bureau on this activity.

The responses from the following nineteen countries were received[10]: Australia, Belgium, Brazil, Canada, Egypt, France, Greece, Hungary, Ireland, Italy, Nepal, Netherlands, Norway, Portugal, Slovakia, Slovenia, United Kingdom, Unites States of America, and Uruguay. The lack of responses from China, Germany, India[11], Japan, New Zealand[12], Puerto Rico, Russia, and Spain were noted as they are represented in the IUPAC Bureau. In addition, the lack of responses from the host countries of the preceding and upcoming IUPAC General Assemblies (Turkey and Korea) was noted.

Questionnaire: content

The replies from the NAOs were diverse rather than tending to any unified opinion either on the proposed definition of the mole or in regards to the current definition or the name of the quantity “amount of substance”. Some 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 “to collect opinions and comments”, if any, by the National Adhering Organizations of IUPAC and was stated in the cover letter.

Of the four questions raised, there was no emerging consensus on the definition of the mole. Opinion on all questions was, in fact, equally divided. From the responses it became evident that (1) an informative description of the quantity (chemical amount) is necessary and (2) the name “amount of substance” has to be revised. Overall, many replies stated the need for a better formulation of what is the quantity “amount of substance”. In addition, numerous technical issues were raised although many of them were deemed irrelevant by this Task Group. All of the received replies are attached as Appendix to these minutes.

[10] An initial response from Cuba was received but the answer to the questionnaire was not received.
[11] A response from India was received but it did not pertain to the questionnaire and further requests for clarification went unnoticed.
[12] An initial response from New Zealand was received but the answer to the questionnaire was not received.

5. CLOSING OF THE MEETING

Before closing the meeting, JM put forward a motion to the Task Group members to endorse, in principle, the proposed definition of the mole as it appears in the Draft 9th SI Brochure (16 Dec 2013). The motion was seconded by ZM and the Task Group members present unanimously voted in favor of the motion.[13] The Task Group approved the proposed definition of the mole only "in principle" because several additions are warranted. First, the Task Group members agreed to recommend changing the quantity name "amount of substance" to "chemical amount". In addition, the Task Group drafted an informative paragraph explaining the nature of the quantity which is currently known by the name "amount of substance" and its relationship with the Avogadro number, the Avogadro constant, and the number of entities. This informative paragraph will be sent to the drafting committee working on the 9th edition of the SI Brochure in order to better complement the normative definition of the mole.

JS closed the meeting at 19:40 in the Saturday evening and the Task Group set out to draft the Technical Report.

Juris Meija
Secretary of the Task Group [Ottawa, February 5, 2015], revised in May 9, 2015 and July 27, 2015

[13] All Task Group members voted with the exception of RW who did not attend the meeting.

APPENDIX

IUPAC Project 2013-048-1-100

(1) Letter sent to IUPAC National Adhering Organizations on June 2014 [3 pages]
(2) Replies received from IUPAC National Adhering Organizations [53 pages]

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A CRITICAL REVIEW OF THE PROPOSED DEFINITIONS OF FUNDAMENTAL CHEMICAL QUANTITIES AND THEIR IMPACT ON CHEMICAL COMMUNITIES

2014/Jun/03

To all Chemical Societies represented by
IUPAC National Adhering Organizations

Dear Sir or Madam:

INTRODUCTION

In light of the proposed revision of the International System of Units (SI) [1], IUPAC has launched a project with the task to provide a Technical Report containing a critical review of the definitions for the quantity amount of substance and its unit, mole, as well as the related unit of the quantity mass. This letter is to collect opinions and comments by the IUPAC National Adhering Organizations (NAOs) which will be reproduced in the aforementioned Technical Report.

HISTORY

In 1971, the 14th General Conference of Weights and Measures resolved to define the mole as “the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12…” In addition, “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.” This is the current definition of the mole [2].

In 2011, the 24th General Conference of Weights and Measures proposed a revision of the SI. As a consequence of this, the redefinition of the mole is necessary and its magnitude will be set “by fixing the numerical value of the Avogadro constant to be equal to exactly 6.022 14X × 10^{23} when it is expressed in the SI unit mol^{-1}.” The symbol X represents one or more additional digits to be added to the numerical value of N_A. This is the proposed new definition of the mole [3].

Mole is the name of the SI base unit (symbol mol) for the base quantity *amount of substance* (symbol *n*) which is defined in IUPAC documents (e.g. IUPAC Green Book, 3rd Edition, 2nd Printing 2008 [4]) using the expression $n = N/N_A$, where N is the number of entities, and N_A is the Avogadro constant. Similarly, the SI Brochure (8th Edition 2006 [2]) provides the following definition of the quantity *amount of substance*:

> "Amount of substance is defined to be proportional to the number of specified elementary entities in a sample, the proportionality constant being a universal constant which is the same for all samples … This constant is called the Avogadro constant, symbol N_A or L … the relation is $n = N/N_A$. … the Avogadro constant has the coherent SI unit reciprocal mole."

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.

Because of external time-constraints, Chemical Societies represented by IUPAC NAOs are asked to reply no later than 2014/October/01. The replies should be drafted on a letterhead, signed, and sent in as a PDF format to mole@iupac.org. The comments will be used towards formulating the IUPAC Technical Report. Those organizations who will reply will be sent an advance draft of the IUPAC Technical Report for further comment and input before submission to *Pure and Applied Chemistry*.

Prof. Dr. Jürgen Stohner FRSC
Chairman of the Task Group

REFERENCES

[1] http://www.bipm.org/en/si/new_si/
[2] http://www.bipm.org/en/si/si_brochure/
[3] http://www.bipm.org/en/CGPM/db/24/1/
[4] http://www.iupac.org/home/publications/e-resources/nomenclature-and-terminology/quantities-units-and-symbols-in-physical-chemistry-green-book.html

NORWAY

Date: Mon, 15 Sep 2014 11:04:55 +0200
From: Harald Walderhaug <harald.walderhaug@kjemi.uio.no>

To Prof. Dr. Jürgen Stohner FRSC
Chairman of the Task Group,

Dear prof. Stohner,

This issue was on the agenda for a meeting of The board of the Norwegian Chemical Society, and we do not have special comments to the Proposed Definition of the Mole - we support the proposition.

On behalf of our Society,
Harald Walderhaug, Prof., University of Oslo, and
Secretary General of the Norwegian Chemical Society.

NETHERLANDS

From: Jan-Willem Toering <jwt@kncv.nl>
To: Mole IUPAC <mole@iupac.org>
Date: Fri, 19 Sep 2014 16:57:47 +0200

Dear Professor Stohner,

On behalf of our most distinguished member of the board of the Royal Netherlands Chemical Society Professor Dr. Jan Apotheker, I hereby send you our reply regarding the proposed definition of the mole.

with kindest regards,
Royal Netherlands Chemical Society

mr.drs. Jan-Willem Toering
Director

Dear Professor Stohner

In reaction to the questionnaire you sent about the definition of the mole I have the following remarks.

On behalf of the KNCV I have consulted several colleagues before answering the questions.

We are not very satisfied with the current definition of the mole. The main reason is that with the current definition the mole is coupled to the unit of mass, the kg. The kg is the sole unit in the S.I. system still coupled to an object.

By fixing Avogadro's number to be a natural constant the mole is directly coupled to a constant that can be determined anywhere in a laboratory, given the right equipment.

The definition is not very clear about one thing though. We consider the mole to be a unit, expressing the number of particles/ entities as a fraction of Avogadro's number.

Defined in this way the mole is a unit comparable to the units dozen and gross.

We look upon 'amount of substance' as a property whose value is expressed in the unit mole, which has as a symbol '*n*'. Again this is not very clearly expressed in the proposed definition.

Generally speaking the property 'amount of substance' is generally referred to as 'number of moles' or 'number of particles. Most people consider it to express the number of particles, but expressed in the unit mole. In that sense the 'mole' is considered to be the link between macroscopic phenomena and the molecular world.

We would therefore suggest simplifying the name of the property to 'amount', thus leaving of the term 'of substance' or calling it 'chemical amount'.

The terms 'amount of substance' or 'chemical amount' are not always applicable, for example when the number of photons is expressed in 'moles'

Whishing you all the best with the work in your taskgroup, I remain

Sincerely,

Jan Apotheker, board member education of the KNCV

CANADA

From: Neil Burford <nburford@uvic.ca>
To: Mole IUPAC <mole@iupac.org>
CC: "jim.tunney@nrc-cnrc.gc.ca" <jim.tunney@nrc-cnrc.gc.ca>,
"randersson@cheminst.ca" <randersson@cheminst.ca>
Subject: RE: Remainder / IUPAC Critical Review of the Proposed Definition of the Mole
Date: Fri, 19 Sep 2014 19:20:19 +0000

Dear Prof. Stohner:

Please find below and attached comments and suggestions from Canadian colleagues regarding the proposed definition of the mole.

Please contact me if you require additional information.

Best wishes,

N

Neil Burford
Department of Chemistry
University of Victoria
P.O. Box 3065, Stn CSC
Victoria, BC V8W 3V6

August 12, 2014

Prof. Neil Burford
Chair, CNC-IUPAC

Dear Dr. Burford:

I am satisfied with the redefinition of the mole and its use in defining amount of substance. There is one aspect of the definition of the mole that I believe is worth considering. I note that, in the current definition, it implies a restriction of the use of the mole to the counting of elementary entities. One of the challenges faced by students who first embark on the study of chemical science, is a view that the mole is a special kind of counting unit that (in their minds) might be subject to different arithmetical rules because of this special status and they approach its use with trepidation.

This problem becomes significant in the study of thermodynamics. In all first year chemistry textbooks, we will see written

$$N_2(g) + 3\,H_2(g) \rightarrow 2\,NH_3(g) \qquad \Delta H^\circ = -92.38\ kJ\ mol^{-1}$$

Students often stumble at this point when they ask "What does the 'per mole' refer to? Which entity is 'per mole'?" I am surprised at how this apparent problem is not restricted to students. More than half of the first year chemistry textbooks on my shelves *agree* with the students that there *is* a problem and in response completely drop "mol^{-1}", providing instead just -92.38 kJ and then in the text dictate that this value is applicable only when the stoichiometric coefficients are interpreted as moles. This same "problem" extends to entropy, free energy, and so forth. But in the same textbook in subsequent chapters, when the calculation of, for instance, an equilibrium constant from a standard free energy is undertaken, "magically" the "per mole" reappears – only because it must in order to cancel the "per mole" that forms the definition of the gas constant R. This loose usage of the mole is poor pedagogy and contributes to student perceptions of chemistry as unfathomable.

I contend that the root of this confusion lies in the implied definition that the mole only counts microscopic entities. The solution to the perceived problem above is to realize that the chemist has dropped the necessary explanation of "per mole" in the above chemical equation. In completeness it should read

$$N_2(g) + 3\,H_2(g) \rightarrow 2\,NH_3(g) \qquad \Delta H^\circ = -92.38\ kJ\ (mol\ of\ reaction\ events)^{-1}$$

In all thermochemical equations, the mole is used to count chemical *processes*, not just microscopic *entities*. The stoichiometric relationship

$$\frac{1\ mol\ of\ reaction\ events}{3\ mol\ H_2}$$

can then be used to answer the question of enthalpy released per mole of H_2 consumed. But the key point of understanding is to realize that the thermodynamic values always refer to "per mole of reaction events as written in the chemical equation".

I suggest that the new definition of the mole include the clarification that it is used to count <u>processes</u> involving these elementary entities and not just the entities themselves. The current definition, which according to your letter states "…or specified groups of such particles", is inadequate. A "group" of 1 mole of N_2, 3 moles of H_2, and 2 moles of NH_3 does NOT, by itself, release 92.38 kJ of heat. It is only when 1 mole of N_2 and 3

moles of H_2 *react* to form 2 moles of NH_3 that that amount of enthalpy is released in the form of heat.

I have battled this misconception with students and colleagues for two decades and I hope that a slight, but meaningful, adjustment to the definition of the mole could help to clarify this common source of confusion.

Yours respectfully,

Dan Thomas
Associate Professor
Department of Chemistry
University of Guelph.

EGYPT

Date: Sat, 20 Sep 2014 07:34:11 -0700
From: nadia kandil <nadiaghk@yahoo.com>
Reply-To: nadia kandil <nadiaghk@yahoo.com>
Subject: Re: Remainder / IUPAC Critical Review of the Proposed Definition of the Mole
To: Mole IUPAC <mole@iupac.org>

Dear Prof.Dr. Jurgen Stohner FRSC,

Thank you for your mail. we received your letter and the questionnaire and Paul De Bie`vre's article in June 2014. We discussed it in many Egyptian chemistry groups and in the national committee of Pure and Applied Chemistry and we received from many groups the following answers:

1.Yes ,satisfied with the current definition of the mole.
2.Yes ,satisfied with the current definition of the quantity amount of substance.
3.Yes,satisfied with the current name of the quantity amount of substance.

Best wishes
Nadia

Prof.Nadia.G.Kandile
Titular Member IUPAC
Chairman of the National Committee of Pure and Applied Chemistry
Member of the Promotion Committee of Prof. and Assi.Prof (Organic Chemistry2015)
Prof.of Applied organic Chemistry,Chemistry Department, Faculty of Women
Ain Shams University,Heliopolis ,Cairo,Egypt.
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Mobile :- +201222260339

PORTUGAL

Date: Fri, 26 Sep 2014 11:37:32 +0100
Subject: Project 20!3-048-1-100 -SPQ-Portugal
From: Maria Clara Magalhães <mclara@ua.pt>
To: <mole@iupac.org>

Dear Prof. Dr. Jürgen Stohner
Enclosed as attachment you can find the participation in your questionnaire from the Portuguese Chemical Society.
I hope we can participate more deeply in this discussion once it is a matter of big importance not only to the chemists but to a very broad spectrum of the society. Changes of definitions do not have great impact in the society , if the value will not change, but changes of name can have severe economical implications.
Yours sincerely
Clara Magalhães

Prof. Dr. Clara Magalhães
Chair, SSED, IUPAC

Department of Chemistry and CICECO
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T:+351 234 401518
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SOCIEDADE PORTUGUESA DE QUÍMICA

Portuguese Chemical Society - IUPAC Portuguese Adhering Organization

About the new definitions for the quantity *amount of substance* and its unit the mole

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.

No.

Following the general rule that the SI base units must be defined by themselves, it is understandable the need for changing the definition of the unit mole that, in its current format, makes use of another SI base unit, the kilogram.

The kilogram is the only base unit defined by a prototype. As a median difference of 25 micrograms along one hundred years was evidenced, it was suggested to better assure its long-term stability by adopting a new definition referenced to a fundamental constant. Rewordings of the definitions of all base units were concomitantly and coherently suggested by reference to given fundamental constants. It is expectable such a rewording for the definition of the mole.

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.

Yes.

If the definition will be as written in the *Draft of the 9th SI brochure*:

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 6.022 141 29 x 10^{23} when it is expressed in the SI unit mol^{-1}.

We agree with this definition, in the way it is written in this text.

Indeed, in the current definition of the mole, the sentence "…*a system which contains as many elementary entities as there are atoms in* 0.012 *kilogram of carbon* 12…" has already implicit the numerical value 6.022 14X × 10^{23} that is the one of the Avogadro constant and that is then the fundamental constant of the new definition of the mole.

SOCIEDADE PORTUGUESA DE QUÍMICA

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.

Yes.
The current definition of the amount of substance is the following:

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. The proportionality constant is the reciprocal of the Avogadro constant N_A, so that $n = N/N_A$. The unit of amount of substance is called the *mole*, symbol mol.

This definition satisfies us.

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.

No.

In the 3rd edition of the Green Book, page 4, it is recommended that *"The physical quantity "amount of substance" should no longer be called "number of moles" …".* Therefore, there is a need to take advantage of the new definition of the quantity "amount of substance" and of its unit "the mole" to update its name, as it has been in discussion, for some years, in the community of chemists. However, some of us do not agree changing the name to "number of entities", arguing that a number cannot be a unit, independently on the entity. For instance, the Avogadro constant bridges the macroscopic world with the atomic size world.

Once, there is no consensus in the scientific community, at the moment, we only support the definition of mole as given in the *Draft of the 9th SI brochure*. Any definition that will substitute the term "amount of substance" by any other one will not be supported by the Portuguese Chemical Society. Indeed, the change of the name of the physical quantity is a subject that still needs a further and deeper discussion inside the scientific community.

Portugal, 25th September 2014

Clara Magalhães

Maria Clara F. Magalhães
(On behalf of the Portuguese Chemical Society)

P. S. This document was built with the collaboration of Carlos Corrêa and Olivier Pellegrino.

SLOVAKIA

Date: Fri, 26 Sep 2014 14:05:00 +0200 (CEST)
From: Milan Drabik <Milan.Drabik@savba.sk>
To: Mole IUPAC <mole@iupac.org>
Cc: Fabienne Meyers <fabienne@iupac.org>
Subject: Re: Remainder / IUPAC Critical Review of the Proposed Definition of the Mole

Dear Prof. Stohner & everyone concerned,

Find attached the feedback representing the opinion of chemists
from Slovakia upon “the issue of the redefinition of mole”.

My best regards , Milan Drabik.

Assoc. Prof. RNDr. Milan DRÁBIK, PhD.
E-mails: drabik@fns.uniba.sk, uachmdra@savba.sk

Chairman of the Slovak National Committee of IUPAC
T. M. of the Inorganic Chemistry Division of IUPAC
A.M. & D.R. to the ICTSN of IUPAC (new)
Member of the Divisions (Inorganic Chemistry, Solid State & Materials Chemistry) of EuCheMS
Life-member, Institute of Materials (IoM), U. K.
Life-member, Slovak Chemical Society (SCHS), Slovakia

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SLOVAK REPUBLIC Fax : +421-2-59410444
http://www.uach.sav.sk/

To: **i) Prof. Dr. Jurgen Stohner, FRSC, Chairman**
ii) The entire Task Group

The feedback of chemists from Slovakia upon the distributed Questionnaire is summarised below.

Question No.	**Reply**
1.	NO

b. i) The value of Avogadro constant – N(A), including its uncertainty, should be given in the definition.

ii) In topical case of the definition of the mole: 12C and the dependence of the mole upon the kilogram would be overcome if the Avogadro constant accepted as one of the seven defining constants.

c) To give the exact value of N(A).

2.	YES
3.	YES
4.	YES

May I, representing the members of the Slovak National Committee of IUPAC and the Slovak Chemical Society (Slovenská chemická spoločnosť), add and conclude as follows. The feedback of chemists from Slovakia upon both the distributed Questionnaire and the texts (chpts. 2.2, 2.4.6, 2.4.8, 2.5.6 and Table 2) on "SI unit of amount of substance, the mol" in (http://www.bipm.org/utils/common/pdf/si_brochure_draft_ch123.pdf) – the "Draft 9th SI Brochure", are reflected. The proposed new definition of the mole and also the issue that value of the Avogadro constant proposed as one of the seven defining constants (both no longer dependent on the definition of the mass and kilogram) exert "an easy-to-follow language". "Lower visibility" of unified atomic mass constant is a subsequent drawback, if the motion will get topical. Anyway, the use of the mole and related terms, incl. unified atomic mass constant, by the community of chemistry practitioners (and properly educated students) in Slovakia may continue with the advantage.

Signed

By: ***Assoc. Prof. Milan Drabik PhD,***
Chairman of the Slovak National Committee of IUPAC (Predseda SNK IUPAC),
TM of the Division II of IUPAC, AM of the ICTNS of IUPAC

In: ***Bratislava, Slovakia***

On: ***September 26th , 2014***

ΕΝΩΣΗ ΕΛΛΗΝΩΝ
ΧΗΜΙΚΩΝ

Ν. Π. Δ. Δ. Ν. 1804/1988
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Athens, September 29th 2014
Ref. Number 790

Prof. Jürgen Stohner

Chairman of the Task Group

Zürich University of Applied Sciences

Institute for Chemistry & Biological Chemistry (ICBC)

Campus Reidbach RC E0.40,

Einsiedlerstrasse 31,

CH-8820 Wädenswil

Switzerland

Subject: A CRITICAL REVIEW OF THE PROPOSED DEFINITIONS OF FUNDAMENTAL CHEMICAL QUANTITIES AND THEIR IMPACT ON CHEMICAL COMMUNITIES (2014/Jun/03)

Dear Professor Stohner,

The Association of Greek Chemists (AGC), the NAO representing the Greek community of Chemists in IUPAC, is replying to you due to the proposed definitions of the mole.

The Association of Greek Chemists set up a committee consisting of the Professor of Analytical Chemistry M.I. Karayannis, Professor of General and Inorganic Chemistry N. Klouras, the school counselor of Chemistry. Dr A. Mavropoulos and the representative of the Executive Committee of the AGC, Mrs F. Sideri, which studied the proposed by the IUPAC changes and the relevant discussions in the literature and

concluded the following in respect to the questions:

Number	Answer	Justification
1	NO	The new definition of mole will be consistent with the particulate nature of matter, thus the proposed definition releases the concept of mole from the concept of amount of substance and relates it directly to the number of entities. A Dalton is defined as 1/12th of the mass of a single ^{12}C atom. Together with the fixed value of the Avogadro constant, the Dalton will serve to redefine the kilogram in a way that would suit the needs of the chemists (kg= the mass of 6.02214X..YZ.10^{23} atoms of ^{12}C, multiplied by 1000/12.
2	YES	
3	NO	Because the Avogadro's number is not fundamental or a true invariant constant throughout *time* and *space,* therefore its numerical value must be fixed explicitly before it can be used for the definition of the quantity amount of substance. A new definition, will not only lead to a more instructive term but also to the clarification of the underlying concept.
4	YES	

The AGC is working on strengthening its ties with IUPAC, both in participation and nationwide dissemination of IUPAC information. Any help from you would be really appreciated.

We are always at your disposal in order to answer questions and participate in IUPAC tasks and matters. We wish you good luck in your mission.

Yours sincerely,

For the Executive Committee of the AGC

The President **The Secretary**

Dr. A. Papadopoulos **M. Stratigakis**

URUGUAY

Date: Mon, 29 Sep 2014 15:24:25 -0300
To: Mole IUPAC <mole@iupac.org>
From: Gabriela Garcia <gabig@fq.edu.uy>
Subject: Re: Remainder / IUPAC Critical Review of the Proposed Definition of the Mole

Dear Prof. Stohner,
Please, find below the answers to the questionnaire.

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?

Yes. From a chemical point of view, the current definition of mole is satisfactory. Essentially, this definition follows the chemical line of thought that J. Dalton initiated.

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?

Yes, if it is a necessary change to bring the mole into line with other SI units definitions. Nevertheless, it will lose its chemical identity.

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?

Yes.

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?

Yes.

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.

Thanks!

Best regards,
Gabriela Garcia
PEDECIBA QUIMICA

BRAZIL

Date: Tue, 30 Sep 2014 02:31:47 -0300
From: "Adriano D. Andricopulo" <aandrico@ifsc.usp.br>
To: mole@iupac.org
CC: Diretoria-SBQ <diretoria@sbq.org.br>, "Vanderlan da S. Bolzani" <bolzaniv@iq.unesp.br>,
"Adriano D. Andricopulo" <aandrico@ifsc.usp.br>
Subject: Re: Enc: Critical Review of the Proposed Definition of the Mole

Dear Prof. Jürgen Stohner,

Please find enclosed a contribution of the IUPAC NAO of Brazil (Brazilian Chemical Society) to this important project.

Best regards,

Adriano D. Andricopulo
President of the Brazilian Chemical Society

Vanderlan da S. Bolzani
Representative, IUPAC NAO of Brazil

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?
ANSWER: **NO**

b. If NO, please specify in a few sentences why you opted for NO.
ANSWER: It would be better to refer directly to the Avogadro number instead of the convoluted reference to it by "as many entities as there are atoms in 12 g of C-12".

c. If NO, please provide some suggestion on what to change.
ANSWER: Please see reply to question 4 below.

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 Measurements?

a. YES or NO?
ANSWER: **NO**

b. If NO, please specify in a few sentences why you opted for NO.
ANSWER: What is referred to as a new definition of the mole is actually only a statement that its magnitude will be set by fixing the Avogadro number to 6.022 14X $\times$ 10^{23}. This is not a clear definition of the mole.

c. If NO, please provide some suggestion on what to change.
ANSWER: Please see reply to question 4 below.

3. Are you (as NAO representing your members) satisfied with the current definition of the quantity amount of substance?

a. YES or NO?
ANSWER: **NO**

b. If NO, please specify in a few sentences why you opted for NO.
ANSWER: The current definition of the quantity "amount of substance" (IUPAC GOLD BOOK: "the number of elementary entities divided by the Avogadro constant") is not really a definition; it is simply a way of calculating its value in moles, for a given sample of entities (a similar awkward situation would be to define the volume of a given sample as "the mass of the sample divided by its density"). This situation is a consequence that the term "amount of substance" originally was not a good choice to convey the quantity measured in moles (see e.g. Milton and Mills [1]), mostly because it does not clearly convey an underlying concept.

c. If NO, please provide some suggestion on what to change.
ANSWER: The expression "amount of substance" needs to be replaced by one that embodies a clearly stated underlying concept. Then the definition of the quantity will be easily understood and independent of the way its value is calculated.

4. Are you (as NAO representing your members) satisfied with the current name of the quantity amount of substance?

a. YES or NO?

ANSWER: **NO**

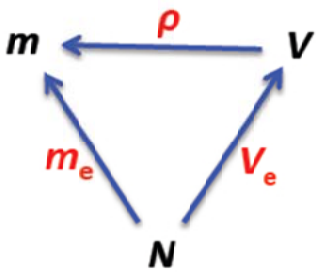
b. If NO, please specify in a few sentences why you opted for NO.

ANSWER: First of all, we think that the question is not properly formulated. It should be "Are you satisfied with the current name for the SI base quantity whose SI base unit is the mole?" Our answer is no for the reasons already stated in our answers to question 3.

c. If NO, please provide some suggestion on what to change.

ANSWER: We suggest that "numerosity" might be the proper name for the SI base quantity whose SI base unit is the mole. Actually a Brazilian chemist, Romeu C. Rocha-Filho, first put this suggestion forward in an article published in 1988 (in Portuguese) in our NAO's journal *Química Nova* [2] (a preliminary version of the suggestion was presented as a poster at IUPAC's 8^{th} *International Conference on Chemical Education* [3]). Two years later he had the same proposition published in the *Journal of Chemical Education* [4], and more recently he reproposed it in the journal *Accreditation and Quality Assurance* [5]; see also De Bièvre's recent paper [6]. Hereinafter, a summary of the reasoning underlying this proposal will be presented.

From a macroscopic (continuous) point of view, the quantity of a given substance in lab-scale samples can be expressed either through their mass (m) or their volume (V). An additional way of expressing the quantity of the given substance in the lab-scale samples is stating the number (N) of entities (atoms, molecules or formula units) contained in the samples; this is a microscopic (discontinuous) point of view that, although chemically sensible (stoichiometry involves relationships between numbers of entities), leads to the cumbersomeness of dealing with very large values of N (coupled to very small values of mass and volume, i.e. the mass and volume of the entities contained in the samples: m_e and V_e, respectively) – this problem was previously highlighted by others (e.g. McGlashan [6]). The following diagram shows the relationships between these quantities, where ρ is the mass density.



i.e.: $m = \rho \times V$, $m = m_e \times N$, and $V = V_e \times N$. From this diagram, it is clear that $m_e = V_e \times \rho$.

About 130–140 years ago, chemists started using a clever, alternative way of indirectly dealing with this problem, i.e. working with multiple or submultiple values of a fixed value of N, the Avogadro number (N_0) of entities contained in certain special values of the mass of the samples: atom-grams or molecule-grams (today's molar masses, M). This was simply a way of

controlling how numerous in given entities each sample of a substance is, since this is what is important from the stoichiometric point of view.

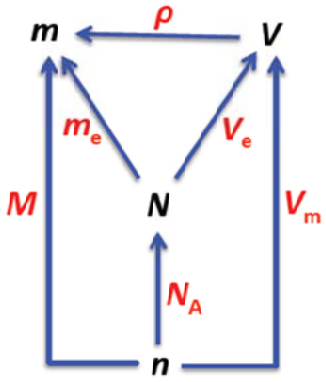
Considering that:

a) the value of N_0 is being set as exactly equal to 6.022 14X $\times 10^{23}$;
b) a sample that contains a large number of entities has the associated attribute of being "numerous";
c) the quality of being numerous or many is referred to as "numerosity";
d) to each given number of entities one may associate a given numerosity,

it is proposed that the numerosity (n) associated to N_0 entities be defined as equal to 1 mole exactly, i.e.:

"The mole is the numerosity of a sample of entities numbering exactly N_0".

One important idea underlies this proposal, i.e. that the mole plays a role similar to that of the dozen, the gross or the ream for samples of much smaller numerosities, i.e. the dozen, gross, and ream are other possible units of numerosity (then, "the dozen / gross / ream is the numerosity of a sample of entities numbering exactly 12 / 114 / 500") – many other such units can be defined if necessary and useful. In this sense, clearly the mole can be seen as being "science's dozen" (an understanding that has been present in textbooks and in the educational literature for quite some time – see e.g. Kolb [8]). The following diagram shows the relationships between m, V, N, and n, where V_m is the molar volume and N_A (= N_0 mol^{-1}) the Avogadro constant.



i.e.: $N = N_A \times n$, $m = M \times n$, and $V = V_m \times n$. From this diagram, it is clear that $M = N_A \times m_e = V_m \times \rho$ and that $V_m = N_A \times V_e$.

Considering that the redefinition of the kilogram is closely related to that of the mole (with possible very significant implications), here it is important to note that we also propose that the "atomic kilogram" be chosen instead of the "electronic kilogram" (see Hill *et al.* [9]), because that makes much more sense from a chemical and educational point of view (see Hill [10]). Then, the mass associated to N_0/0.012 atoms of carbon-12 is defined as equal to 1 kilogram exactly, i.e.:

"The kilogram is the mass of N_0/0.012 unbound atoms of C-12 at rest and in their ground state".

The main idea that underlies this proposal is that N_0 is thus associated to an exact mass of carbon-12, i.e., 12 g, with the consequence that 1 g = N_0 u or 1 g = N_0 Da, considering that 1 u = 1 Da.

The proposals presented hereinbefore reconcile rigorous scientific and metrological aspects with educational/pedagogical aspects, making the mole and the kilogram much more easily understood. Thus, the Brazilian Chemical Society strongly advocates their adoption.

References

[1] M. Milton, I. Mills. “Amount of substance and the mole”. *Chimia*, vol. 63, p. 613–615, 2009.

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[3] R.C. Rocha-Filho. “Proposition of a new definition for the mole unit”. *The Eighth International Conference on Chemical Education*. IUPAC/Chemical Society of Japan, Tokyo, 1985. Book of Abstracts, p. 167.

[4] R.C. Rocha-Filho. “A proposition about the quantity of which mole is the SI unit”. *Journal of Chemical Education*, vol. 67, p. 139–140, 1990. DOI: 10.1021/ed067p139.

[5] R.C. Rocha-Filho. “Reproposition of numerosity as the SI base quantity whose unit is the mole”. *Accreditation and Quality Assurance*, vol. 16, p. 155–159, 2011. DOI: 10.1007/s00769-011-0752-7.

[6] P. De Bièvre. “CCQM owes chemists a description of the concept ‘amount of substance’”. *Accreditation and Quality Assurance*, vol. 19, p. 323–325, 2014. DOI: 10.1007/s00769-014-1068-1.

[7] M.L. McGlashan. “Amount of substance and the mole”. *Metrologia*, vol. 31, p. 447–455, 1994/1995. DOI: 10.1088/0026-1394/31/6/004.

[8] D. Kolb. “The mole”. *Journal of Chemical Education*, vol. 55, p. 728–732, 1978. DOI: 10.1021/ed055p728.

[9] T.P. Hill, J. Miller, A.C. Censullo. “Towards a better definition of the kilogram”. *Metrologia*, vol. 48, p. 83–86, 2011. DOI: 10.1088/0026-1394/48/3/002.

[10] T.P. Hill. “The kilogram kabal”. *The Chronicle Review*. 6 July 2012, p. B4.

São Paulo, September 30, 2014.

Adriano D. Andricopulo

President, ***Brazilian Chemical Society***

Vanderlan da S. Bolzani

Representative, ***IUPAC NAO of Brazil***

AUSTRALIA

From: Robyn Taylor <robyn.taylor@raci.org.au>
To: "mole@iupac.org" <mole@iupac.org>
Date: Tue, 30 Sep 2014 16:52:23 +1000
Subject: Proposed Definitions Review Questionnaire

Dear Prof Stohner

Please find attached the RACI's response to the Questionnaire Re: A Critical Review of the Proposed Definitions of Fundamental Chemical Quantities and their Impact on Chemical Communities.

On behalf of: Professor Mark Buntine FRACI CChem

President RACI

Email: m.buntine@curtin.edu.au

Kind Regards

Robyn Taylor

RACI – Administration

NATIONAL OFFICE

The Royal Australian Chemical Institute Inc.
1/21 Vale Street, North Melbourne, Victoria 3051 Australia
Phone: +61(0) 3 9328 2033 Fax: +61 (0) 3 9328 2670
Email: robyn.taylor@raci.org.au. http://www.raci.org.au/

Royal Australian Chemical Institute

30 September 2014

International Union of Pure and Applied Chemistry
IUPAC Secretariat
PO Box 13757
Research Triangle Park, NC 27709 USA

Email: mole@iupac.org

Dear Sir/Madam

RE: A CRITICAL REVIEW OF THE PROPOSED DEFINITIONS OF FUNDAMENTAL CHEMICAL QUANTITIES AND THEIR IMPACT ON CHEMICAL COMMUNITIES

Our response to the questions asked in the questionnaire are:

1. YES - we are happy with the current definition but understand why the redefinition is required in light of the broader changes that are occurring to the SI.

2. YES - but we note that the definition of the mole as "the SI unit of substance of a specified elementary entity, which may be an atom, …. or a specified group of particles" needs to be extended to allow for reaction equations. Thus, specifically, the Green Book, 3rd ed., p. 58, note (15) requires that the reaction must be specified for which reaction enthalpy (SI unit: J mol-1) is reported. So, there is a need to include "a mole of reaction" in the definition

3. YES

4. NO - We find the term 'quantity of substance' confusing for those not used to it and prefer the term 'chemical amount', with the mole to be recognised as the unit of chemical amount. However, we also recognise that this term ignores the many other users of the quantity in eg the biological field so great care is needed with a replacement to ensure it is more understandable but also captures all users of the quantity

Yours sincerely

Professor Mark Buntine FRACI CChem
President RACI

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HUNGARY

From: george.horvai@mail.bme.hu
Date: Tue, 30 Sep 2014 12:53:06 +0200
To: mole@iupac.org
Cc: Juergen Stohner <sthj@zhaw.ch>, Erno Keszei <keszei@chem.elte.hu>

Dear Colleagues,

Please find attached our filled in questionnaire.

Our response was worked out mainly by professor Erno Keszei, Roland Eotvos University, Budapest, keszei@chem.elte.hu.

Yours

George Horvai

QUESTIONNAIRE (Response of the Hungarian NAO) 30 September 2014

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.

In fact, it depends on the actual value of the SI unit kg, thus it is subject to change with time, which makes values of experimentally determined molar quantities for different substances become obsolete, simply due to the fact that the quantity 1 kg changes. (A good example for such discrepancy is standard pressure defined previously as 1 atm or recently as 10^5 Pa.)

c. If NO, please provide some suggestion on what to change.

The present proposal (Draft 9th Brochure 16 December 2013) is reasonable and acceptable.

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.

Nevertheless, ***there is a problem with a related definition: the molar mass***. We find the present (and in the brochure proposed) definition of the molar mass too much confusing. A logical definition would be "the mass of one mol of entities", instead of keeping the relative mass to a fixed amount of C^{12} isotopes.

Thus we suggest that the definition of the molar mass should simply be the mass of one mole of entities. (We know that it is not the subject of the CGPM but rather the IUPAC and IUPAP, but they should formulate a similar recommendation to CGPM before the final improvement of the new SI statement.)

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.

The current definition invokes mass. On one hand, it depends on the actual definition of the SI unit kg – which, as was the case a few times, is subject to change. On the other hand, the quantity "amount of substance" expresses simply ***numerousness***, (N_A entity of something), which has nothing to do, and should not depend on mass.

c. If NO, please provide some suggestion on what to change.

The present proposal (Draft 9th Brochure 16 December 2013) is reasonable and acceptable.

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.

The present proposal (Draft 9th Brochure 16 December 2013) – at several instances explicitly, at some others implicitly – makes it clear that the "amount (of substance)" is simply the numerousness of any entities ($6.022\ 141\ 29 \times 10^{23}$ of them). The word "amount" is correct to express this notion, just like we can say "three hundreds" of them, which refers to amount. (The French usage is even more explicit: trois centaine.) However, numerousness is not restricted to chemical entities only. In fact, if we give reaction energies (enthalpies, entropies, etc.) in units of kJ/mol or kJ/ (mol K), we always refer to ***1 mol of the stoichiometric equation*** referring to corresponding chemical entities. Similarly, we could count galaxies or stars in the universe in mole units.

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

Taking into account the above arguments, the name of the quantity should reflect this more general meaning of numerousness. (It is not surprising that, out of the seven basic quantities in the SI, the only one is the amount of substance whose unit – i. e. the natural constant it depends on – is independent of any, more precise, future measurements and has a well determined value not to change any more.) A name already suggested (***numerosity***) is a good candidate, but, unfortunately, it does not sound in harmony with the previous name (amount of substance) – though it is not that far from the expression still largely used "number of moles" or "mole number". Linguists and chemists together should find or even ***invent*** a more suitable name. (See "googol" for 1×10^{23}.)

A final remark: speaking of 6.022 141 29 $\times10^{23}$ entities keeps an old convention, but speaking of 1 entity (and any of its multiples) would be more logical. This raises the question of the usefulness of making definitions about countable entities.

ITALY

Date: Tue, 30 Sep 2014 14:51:07 +0200
From: "cecilia.tribuzio" <cecilia.tribuzio@cnr.it>
To: Mole IUPAC <mole@iupac.org>
CC: Tundo <tundop@unive.it>, frpavese@gmail.com
Subject: CNR, Italy - IUPAC Critical Review of the Proposed Definition of the Mole

Dear Prof. Dr. Stohner,

plese find here attached the Italian IUPAC NAO reply regarding the proposed definition of the mole.

Best regards
Cecilia Tribuzio

Consiglio Nazionale delle Ricerche

ITALIAN NATIONAL COMMITTEE FOR IUPAC

Prof. Dr. Jürgen Stohner FRSC
Chairman of the Task Group IUPAC Project 2013-048-1-100 – A Critical Review of the Proposed Definition of Fundamental Chemical Quantities and Thier Impact on Chemical Communities.

Dear Prof. Stohner,

I am pleased to send you in a separate letter the comments to the Questionnaire. They were filed by prof. Franco Pavese - IUPAC Commission I-1 (Green Book), Italian National Representative (formerly Titular Member).
Consiglio Nazionale delle Ricerche, Istituto di Metrologia "G.Colonnetti" (IMGC) and Istituto Nazionale di Ricerca Metrologica (INRIM), Torino.

The Questionnaire was approved by the Italian National Committee for IUPAC, http://www.iupac.cnr.it/.

I will be glad to be informed on the development of your Project.

Sincerely yours,

Pietro Tundo
Professor of Organic Chemistry
Ca' Foscari University of Venice
IUPAC Past- President Division of Organic and Biomolecular Chemistry
President of the Italian National Committee for IUPAC.

Venice, September 30th, 2014

Consiglio Nazionale delle Ricerche

ITALIAN NATIONAL COMMITTEE FOR IUPAC

NAO: Consiglio Nazionale delle Ricerche, ITALY

QUESTIONNAIRE

1. Are you (as NAO representing your members) satisfied with the current definition of the mole?

a. YES or NO? **NO**

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

The present definition resorts to a specific mass, a dependence that is not deemed necessary for this unit, but reserved to the suggested new unit of mass: "The gram, unit of mass, symbol g, is one-twelfth (1/12**) of the mass of** 6.022 14X YZ x 10^{23} **atoms of** ^{12}**C in their nuclear ground state"**

c. If NO, please provide some suggestion on what to change.

The following change is suggested (see also 4.c):
"The mole, unit of the chemical amount (or, alternatively, number of entities), symbol mol**, is a number of entities equal to** 6.022 14XYZ x 10^{23} **entities exactly.**
Note 1: The entities must be specified
Note 2: The Avogadro number is recognised as a scaling factor of individual entities between the macroscopic and the microscopic frames."

Notes
A: 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 or number of entities (see 4.c), and the mole be also recognised as the unit of chemical amount or number of entities;
B: 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.

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? **NO**

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

(NOTE: It was not "proposed by the CGPM in 2011", but the CGPM "took note" of it)

The definition proposed by the CCU of the BIPM uses the inverse of an "Avogadro constant" (or "reciprocal mole"), which brings to basic inconsistencies in the definition and equivocal interpretation of the quantities involved.
The expression "The numerical value is set at … when it is expressed … in units mol^{-1}" is a circular one.

c. If NO, please provide some suggestion on what to change.

The following change is suggested:
"The mole, symbol mol**, is a number of entities equal to** 6.022 14X YZ x 10^{23} **entities exactly**
Note 1: The entities must be specified
Note 2: The Avogadro number is recognised as a scaling factor of individual entities between the macroscopic and the microscopic frames."

Notes
A: 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 or number of entities (see 4.c), and the mole be also recognised as the unit of chemical amount or number of entities;
B: 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.

3. Are you (as NAO representing your members) satisfied with the current definition of the quantity amount of substance?

a. YES or NO? **NO**

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

No introduction of a new quantity is deemed necessary for the unit mole (see previous Note A: "The proposed definition does not require an associated quantity other than 1").
The decision on the issues concerning the quantity should precede the decision on the unit.

c. If NO, please provide some suggestion on what to change.

In order to maintain continuity with the present ISQ, the present quantity amount of substance is renamed "chemical amount" or "number of entities" (see 4.c), and the mole be also recognised as the unit of chemical amount or number of entities (from Note A).

4. Are you (as NAO representing your members) satisfied with the current name of the quantity amount of substance?

a. YES or NO? **NO**

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

<u>Subsidiary to answer 3.b and subordinated to that reply</u>:
(a) the term "amount" in common English language is subject to ambiguity of the meaning, especially when applied to "substance";
(b) "amount of substance", in the meaning intended by the definition of amount of substance, does not match the definition of "quantity" of the International Vocabulary of Metrology (VIM) term (1.1) "property of a phenomenon, body, or substance, where the property has a magnitude that can be expressed as a number and a reference".

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

The following new names are suggested:
"chemical amount" or "number of entities"

IRELAND

From: Rebecca Farrell <R.Farrell@ria.ie>
To: Mole IUPAC <mole@iupac.org>
Subject: RE: Remainder / IUPAC Critical Review of the Proposed Definition of the Mole
Date: Wed, 1 Oct 2014 09:04:14 +0000

Dear IUPAC,

Please find the response from the Royal Irish Academy Physical Chemical and Mathematical Sciences Committee to the below.

I would be most grateful if you could confirm receipt.

Kind regards,

Becky

ROYAL IRISH ACADEMY

Royal Irish Academy Physical, Chemical and Mathematical Sciences Committee - response to IUPAC 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?

   No

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

The current definition is linked to the definition of a kilogram and I would prefer it to be linked to an exact numerical value of Avagadro's constant. The mole, 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, is such that the Avogadro constant is equal to exactly 6.022 141 79 x 10^23 per mole.

c. If NO, please provide some suggestion on what to change.

Suggestion noted above.

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?

Yes

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?

No

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

The current definition is related to the current definition of a mole, so the suggested change is now required.

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? YES

Yes

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.

Professor Pat Guiry MRIA
On behalf of the RIA Physical, Chemical and Mathematical Sciences Committee

UNITED STATES OF AMERICA

On 10/1/14, 2:04 PM, "Hughes, Kathryn" <KHughes@nas.edu> wrote:

Dear Marcy,

Attached please find the response from the American Chemical Society's Nomenclature, Terminology, and Symbols to the questionnaire sent to them by the US NAO. Within the United States, of course, the National Institute of Standards and Technology represents the US government's position. I trust that the IUPAC committee is well aware of the formal international discussion on the topic, and as a result I have not reproduced NIST's position here. If you would like more information on that point, I would be happy to provide it in a follow up email.

I also recently learned that the American Association for Clinical Chemistry also has an interest in the topic, and though the answers will return after your deadline, I will send on any response I receive from that organization for your consideration as well.

Best regards,
Kate

NTS Responses to the IUPAC Questionnaire†

1) Are you satisfied with the current definition of mole?

a) No; however, chemists have lived with it for over 40 years, so they certainly can live with it.

b) "Amount of substance" is a term that is not widely used by practicing chemists nor others in allied chemical fields. (See below under questions 3 & 4.)

c) See 2c below.

2) Are you satisfied with the new definition proposed for the mole?

a) The proposed definition is better than the current one; however, it still refers to the quantity "amount of substance", deemed unsatisfactory even by the BIPM.

b) The proposed definition[1] is closer to the definition given in many introductory chemistry textbooks. The latter tend to define the mole as Avogadro's number[2] of elementary entities. The fixed-constant definition of the mole is closer than the current definition to this current practice in chemical education and chemistry allied fields such as the health professions.

c) The mole need not be included as a unit in the SI and was not until 1971; it will continue to be used by chemists. A definition that reflects widespread usage by chemists and chemistry educators is "The mole contains exactly 6.022 141 29 $\times 10^{23}$ specified entities." [As a practical matter, in the context of chemistry, those entities will be "atoms, molecules, ions, electrons, other particles, or specified groups of such particles" as specified in the current SI Brochure[3].]

3) Are you satisfied with the current definition of amount of substance?

a) No.

b) The current SI Brochure[3] states "The quantity used by chemists to specify the amount of chemical elements or compounds is now called 'amount of substance'. Amount of substance is defined to be proportional to the number of specified elementary entities in a sample, the proportionality constant being a universal constant which is the same for all samples." The IUPAC Gold Book[4] adds "Since it is proportional to the number of entities, the proportionality constant being the reciprocal Avogadro constant and the same for all substances, it has to be treated almost identically with the number of entities." Many chemists and chemistry educators consider the quantity of which mole is a unit to be the number of entities, and they do not observe a distinction between proportionality to and identity with number of identities. Furthermore, the first sentence quoted from the SI Brochure has a serious factual problem: the quantity used by chemists to specify the amount of chemical elements or compounds is ***not*** generally called amount of substance.[5]

c) See 4c below.

4) Are you satisfied with the current name of amount of substance?

a) No.

b) The name is ambiguous. Mass, volume, and number of entities are all measures of the amount or quantity. Whatever the name of this quantity, its determination is commonly made by measurement of mass ('counting by weighing')

c) “Number of entities” is a clearer name for what practicing chemists think the mole measures. If a distinction must be made between a purely numerical quantity (like a dozen or gross) and a quantity that is proportional to number of entities—a distinction chemists and chemistry educators tend not to observe—then a name free from the word “amount” ought to be chosen. After all, the word “amount” is used for different entities in the SI Brochure[3] (“amount of heat” and “amount of electricity” as well as “amount of substance”). If the term “amount of substance” is retained, the option of dropping “of substance” ought not to be countenanced, as it is in the current SI Brochure. (And if “amount of substance” is retained, it is likely to continue to be used by chemists as infrequently as it is today.) And if the term “amount of substance” is retained, then the preferred formulation from Question 2c above would become “One mole is the amount of substance containing exactly 6.022 141 29 $\times 10^{23}$ specified entities.”

The Kilogram

While the input from NTS on the kilogram was not sought at this time, its definition has received much attention from this committee in recent years. The Committee has noted the importance of maintaining the “compatibility condition”[6] that exists in the current SI which links Planck’s constant, Avogadro’s constant, and the mass of the carbon-12 atom.

In its simplest form, this compatibility condition requires that $h\,N_A = K_c M(^{12}C)$, where K_c is a combination of other well-characterized constants. From this relationship, it is clear that any two (and ONLY two) of the three quantities (Planck’s constant, Avogadro’s constant, and the mass of carbon-12) may be fixed. Affirming the carbon-12 atomic mass as exactly 12 would require either h or N_A to be determined experimentally. Fixing N_A would produce a conceptually simple, readily achievable alternative to the proposed definition for the kilogram as $\left(\frac{1000}{12}\right) \times 6.0221014129 \times 10^{23}$ times the mass of an atom of ^{12}C (at rest and in the ground state). Surely the mass of the ^{12}C atom is a true invariant, and one that has served chemists and physicists well as the basis of the unified atomic mass scale.

The proposed indirect definition of the kilogram via the Planck constant seems to us unnecessarily complex in practice, if not in principle, and presents a high hurdle in explaining this definition to the users of the new SI. The early architects of the new SI indicated that any redefinitions should be “readily comprehensible to students in all disciplines”[7]. We are convinced even the strongest proponents of the new SI will agree that this condition has not been met. In contrast, a carbon-12 based kilogram could produce an eminently teachable statement such as: “ Avogadro’s number, or one mole, of carbon-12 atoms has mass of exactly (12/1000) kilograms”.

In addition to these issues, NTS also notes some technological concerns with the currently favored mise en pratique for the kilogram. Those issues have been addressed by others.

Footnotes

† In 2010, the IUPAC Executive Committee formally recommended adoption of the new definitions (Chemistry International vol. 32 no. 1) under examination here, following limited consultation with the user community. The ACS Committee on Nomenclature, Terminology, and Symbols is grateful for this opportunity to contribute on behalf of the American Chemical Society.

[1]Bureau International des Poids et Mesures, *Draft 9th SI Brochure 16 December 2013*, http://www.bipm.org/utils/common/pdf/si_brochure_draft_ch123.pdf

[2]Note that chemical usage in textbooks and in research papers strongly prefers "Avogadro's number" to the "Avogadro constant." A search of pubs.acs.org turned up 1606 research papers published in ACS journals since the year 2000 that contain the phrase "Avogadro constant" or "Avogadro's constant." The comparable number of research articles containing "Avogadro's number" or "Avogadro number" was 6022.

[3]Bureau International des Poids et Mesures, *The International System of Units (SI)*, 8th ed., Organisation Intergouvernementale de la Convention du Mètre, 2006, http://www.bipm.org/utils/common/pdf/si_brochure_8_en.pdf

[4]IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: http://goldbook.iupac.org (2006-) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins. ISBN 0-9678550-9-8. http://goldbook.iupac.org/A00297.html

[5]A search of pubs.acs.org turned up 413 research papers published in ACS journals since the year 2000 that contain the phrase "amount of substance". The comparable number of research articles containing "number of moles" (the term given in the Gold Book as the former name for amount of substance) was 4436.

[6]B. Leonard, *Metrologia* **43**, L3-L5 (2006)

[7]I.M. Mills, P. Mohr, T. Quinn, B. Taylor, and E. Williams, *Metrologia*, **43**, 227-246 (2006)

FRANCE

From: Nicole MOREAU <nj.moreau@free.fr>
Date: October 3, 2014 8:00:43 AM EDT
To: 'Lynn Soby' <lsoby@iupac.org>, 'Enid Weatherwax' <eweatherwax@iupac.org>
Cc: 'Fabienne Meyers' <fabienne@iupac.org>, hellwich.iupac@gmx.de

Definition of the mole.
After its meeting yesterday, the French Committee for Chemistry is not for the new definition of the mole.
See the attached questionnaire and the note written in our meeting.

Is a new definition of the mole necessary?

Ian Mills, Peter Mohr, Terry Quinn, Barry Taylor, and Edwin Williams proposed to give an exact value to the Avogadro constant (Metrologia, 43, 2006, 227). In the same paper it is suggested to give exact values to the Planck constant, to the electron charge, and to the Boltzman constant. The main idea is to define base units so that they are directly linked to those exact constants because they are universal constants of physics. Such a move has been done already for the speed of light and the definition of the meter base unit (17th CGPM, 1983).

However the following remarks are to be made about the Avogadro constant.

First of all the Avogadro constant is not a universal constant of physics. Nothing prevents to give an exact value to the Avogadro constant but not on this base. The Avogadro constant is a proportionality constant which is born from the choice of 1 made by Dalton for the atomic weight of hydrogen, the lightest gas. Then he set up his atomic weight table. If the value 100 for oxygen were taken instead of 16, as suggested by Berzelius for building up the atomic weight table, the number of atoms per mole would have been different from $6.02214129.10^{23}$. The idea of Mills et al. has no **particular** physical meaning, it is an arbitrary choice.

The new mole definition proposed by Mills et al. relates one mole to an exact number of atoms." *The mole is the amount of matter which corresponds exactly to* $6.02214129.10^{23}$ *atoms*". With the choice of an exact Avogadro constant, it is logical and it looks simple. However let us consider the practical application of such a new definition, the "mise en pratique". How an amount of substance expressed in mole can be measured? Nobody unfortunately knows how to count atoms up to 10^{23}. The new definition does not offer any help. Thus what is the solution? Every chemist uses the weighing balance to measure a number of moles. As a consequence it is better logic to use a mass for the mole definition, as it stands in the present definition.

Even more, how to set up the table of atomic mass with the new definition? There is a gap between practice and definition. To fill it since a standard is needed, the value 12 for carbon-12 is chosen. This is precisely the present situation. What have we **practically** won with the new definition and with an exact Avogadro constant, nothing.

Another way to say the same thing is as follows. If one wants to measure a length, a graduated rule is used. If one wants to measure a duration, a chronometer is used. If one wants to measure a mass, a weighing balance is used. If one wants to measure a temperature, a thermometer is used. If one wants to measure an electric intensity, an A-meter is used. But for a substance amount, what do we do? We use a weighing balance. It then looks quite logical to define the unit of substance amount with the help of a mass, not by counting atoms which is not possible.

Some people might then consider that the mole is not a base unit but a derived unit. Such a question is interesting and its discussion would be valuable. Let us also point out that the choice of an exact number of atoms to define the mole base unit means that one atom is a subunit of the mole.

These remarks point out that the proposal of Ian Mills et al. does not bring any practical advantage. The new definition based upon an exact Avogadro constant cannot be directly applied at the laboratory level and for the teaching of the mole.

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* .

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. *NO*
    b. If NO, please specify in a few sentences why you opted for NO. *N is not a Universal constant but a constant of proportionality, since nobody knows how to count atoms in their fundamental state to measure an amount of substance.*
    c. If NO, please provide some suggestion on what to change. *It remains necessary to define 12 for the atomic mass of 12C as it stands today*

3. Are you (as NAO representing your members) satisfied with the current definition of the quantity amount of substance?
    a. *YES*
    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*
    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

About the mole and the amount of substance

(Comments from Jean Rouquerol and Françoise Rouquerol, October 2014)
jean.rouquerol@univ-amu.fr, francoise.rouquerol@univ-amu.fr

1/ Satisfaction about the current definition of the mole

Yes, we are rather satisfied, conceptually:

(a) Because of the full consistency it keeps between the mole (needed by the chemist for his formalism) and the mass (needed by the same chemist in most measurements and applications)
(b) Because of the perfectly whole numbers this definition gives to the atomic mass of the isotopes, which is well in line with the universal character of the periodic table of elements

2/ Feeling about a new definition of the mole relying on a conventional Avogadro constant

We also understand the conceptual interest of fixing the Avogadro constant. Nevertheless, for the reasons above, we are hesitating and are not sure that such a change is needed.

Also, fixing the Avogadro constant at a conventional value will not help the minds understanding that the Avogadro constant is a true constant of nature, as stressed by Ian Mills in his 2010 "Closing coments", in Chemistry International; it would be more pedagogical to continue looking for its best value in case the definition and measurement of the mass are improved…

3/ Feeling about the current definition of the amount of substance

Yes, satisfying

4/ Feeling about the current name of the amount of substance

As well noticed by Ian Mills and Martin Milton in their 2009 paper in Chemistry International, the name "amount of substance" is not well chosen, since the word "amount" has a common dictionary meaning and the additional words "of substance" seem inadequate to imply chemists.

Generally speaking, the "amount" is indeed a most general property of matter. It is "ontological", since it is closely related to the existence of matter. We must admit that, in its common usage, the concept of "amount" includes all extensive aspects of matter. This means that any extensive property of matter allows assessing a special aspect of the amount: mass,

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volume, length, number of elementary entities (divided by N_A to provide the amount of substance after the current definition)…

The fact that the amount can be expressed through various physical quantities is implicitly accepted in chemistry (and in the IUPAC) when we deal with concentrations. Basically, a concentration is indeed the ratio between two amounts:

Amount of a component / Amount of the whole

and it is usual among chemists to measure the above two amounts with help of either a mass, or a volume, or an amount of substance. The outcome is then a "mass fraction", a "volume fraction", a "mole fraction", a "mass concentration" or still a "mole concentration"…

In other words, it is probably unfair that we chemists hijack the general term "*amount of substance*" by giving it a definition which essentially suits us. Also, we know that such a term lends itself to some misunderstanding. In reality, there are other possibilities, for instance:

a) The "*chemical amount*", again quoted by Ian Mills and Martin Milton, which clearly indicates the field for which this quantity was devised
b) The "*mole amount*" which includes an additional information
c) The "*mole content"* when a piece of substance is considered (a grain, a tablet, a liquid in a container…)
d) The "*elementary amount*" and the "*elementary content*" in case we prefer not to see the name of the unit, the mole, in the term designating the quantity; "elementary" refers here to the elementary entities on which the definition of this amount is based, whatever the unit finally chosen
e) The "*entity amount*" as an alternative to elementary amount and also well in line with the current definition of the amount of substance

The terms above should normally suit the chemists, are relatively easy to understand and leave open the possibility for other scientists or engineers to continue using the mass or the volume to evaluate different types of amounts…as was done by mankind since ages, i.e. since the very beginning of commerce. In some respect, we would not cut ourselves from the rest of the world…

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SLOVENIA

From: Slavko Kaucic <slavko.kaucic@KI.si>
To: "mole@IUPAC" <mole@iupac.org>
Subject: RE: Critical Review of the Proposed Definition of the Mole
Date: Mon, 6 Oct 2014 12:44:05 +0000

Dear Professor Stohner,

please find attached the letter from the Slovenian Chemical Society on the critical Review of the Proposed Definition of the Mole.

I appologise for my late response, but in September I organised two European

Conferences in Slovenia and was very bussy.

With kind regards,

Venceslav Kaucic

Professor Em. Venčeslav Kaučič

President of the Slovenian Chemical Society
Vice-CEO of ENMIX – European Nanoporous Materials Institute of Excellence

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Venčeslav Kaučič
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6th October 2014

RE: Project on a critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities

Dear Professor Stohner,

Slovenian Chemical Society fully andorse your endeavours to provide a Technical Report containing a critical review of the definitions for the quantity amount of substance and its unit, mole, as well as the related unit of the quantity mass.

Slovenian Chemical Society wishes to you and the Task Group a successful and fruitful work.

With kind regards.

Venčeslav Kaučič

President
Slovenian Chemical Society

BELGIUM

On 31/10/14 15:03, "Baekelmans, Paul" <paul.baekelmans@solvay.com> wrote:

Dear Professor Stohner,

I am back from London where I attended a very instructive COCI meeting .
You will find here enclosed the final version of the "mole definition" proposal by our NAO (Belgium)

Considering that we should have in mind that:

- the new definition must be an qualitative improvement of the existing one.
- the new definition must be understood easily by students and should be used daily by the whole community of chemists
- easy to teach.

We hope the definition suggested here under will match these requirements.

Please do not hesitate to contact us.
Dr. Paul Baekelmans
President
National Committee Chemistry Belgium
Best regards

Paul Baekelmans

REPLY OF THE NAO BELGIUM TO IUPAC

General remarks:

1. **IUPAC should be commended for initiating a thorough internal and external consultation (that includes examining the literature) after the first one failed to be organized.**
2. **Scientific problems and issues such as these under examination here, should be taken up by the relevant expert committees and Commissions of IUPAC, in this case: the Analytical Chemistry Division, the Inorganic Chemistry Division (because it hosts the Commission on Atomic Weights), and the Division on Human Health (because chemical measurements for worldwide use have been structured for their measurement units in that Division -in cooperation with IFCC- much more (and better) than in other fields of chemistry. Hence, more authoritative knowledge is already available there.**
3. **It is not for NAOs to give scientific opinions. IUPAC should consult its scientific members and other authorities in the fields such as specialists on terminology and definitions, philosophers of science, and measurement who have demonstrated their expertise by publications.**
4. **Decisions such as on topics here concerned, should not be taken on a voting basis (the working tool of NAOs, e.g., in Council) but on consistent scientific argumentation in the literature.**
5. **Note: "Members" cannot possibly mean all or most of the chemists in an NAO's country.**

The present definition and current proposal of a new definition read as follows:

Present definition, dating back to 1971:

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.*

Current proposal of a new definition

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 YZ • 10^{23} when it is expressed in the unit mol^{-1}"

THE QUESTIONS ADDRESSED TO THE NAOs:

1. Are you (as NAO representing your members) satisfied with the current definition of the mole?

a. YES or NO? **NO**

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

The current definition links a unit mole, widely perceived by practicing analytical chemists as a number, to the quantity mass. Mass and numbers are basically different quantities (applicable to continuums resp. discrete "entities").

In addition –as described in detail in the literature- the unit mole has been used in different interpretations internationally, thus raising a problem of identical "teachability" in schools, undergraduate and graduate university studies, and countries, as well as in across border understanding in trade.

The official definition is thereby basically ignored.

c. If NO, please provide some suggestion on what to change.

We support the definitions proposed by ACD and CIAAW which are easy to understand for anybody interested in common (SI) units, especially in primary, secondary and technical schools where education in (SI) units starts.

The ACD /CIAAW recommend the following future definition of the mole:

The mole, symbol 'mol', is a number of entities equal to 6.022 14X YZ • 10^{23} entities exactly.

Note: The proposed definition does not require an associated unit other than 1.

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? **NO**

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

The reciprocal of a number is not a good unit for a number (of entities). Besides, a unit mol^{-1} presupposes a knowledge of what is the mole. That seems to be a circular reasoning.A definition should be direct and state what it defines without conditions attached.

Note: The CGPM does not propose, but takes note of proposals by CIPM, eventually (dis)approving them.

c. If NO, please provide some suggestion on what to change.

We support the proposals of the IUPAC bodies ACD and CIAAW in that they define directly a specified (integer) number (of entities) to be the unit for numbers (of entities). That number is known by the practicing analytical chemist as the Avogadro number and links the atomic to the macroscopic world. It is determined by measuring the ratio of the volume of one mole (of Si in a Si single crystal) to the volume of one atom (of Si).

3. Are you (as NAO representing your members) satisfied with the current definition of the quantity amount of substance?

The above questions 1 and 2 should logically come after -not precede- questions 3 and 4 since a unit can only be defined when we commonly understand sufficiently enough the quantity to which the unit is allocated.

Notes

The current definition is (SI Brochure 8th edition) is:

Amount of substance is defined to be proportional to the number of specified elementary entities in a sample, the proportionality constant being a universal constant which is the same for all samples. This constant is called the Avogadro constant, symbol N_A or L. … the relation is $n = N/N_A$ … the Avogadro constant has the coherent unit reciprocal mole.

The proposal for a new definition is:

None, meaning that the old one is still used.

a. YES or NO? **NO**

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

A direct, formally agreed, description of what amount of substance really means, apparently is very difficult since such a satisfactory description does not seem to be available as uniquely accepted and applied in the literature and in teaching. That should be realized before a unit can be allocated it. The responsible body for the concept quantity is the ISO Committee TC 12, but, IUPAC can make a good proposal.

The Consultative Committee on amount of substance to the International Committee on Weights and Measures, although having amount of substance in its name (and hence in its tasks), has -so far and remarkably enough- not given such a description of what is central to its task, thereby illustrating the problem with the absence of a commonly accepted name. IUPAC should request that opinion.

Both ISO TC12 and CCQM should first thus provide such a name thus furnishing the necessary basis for any redefinition of the unit going with this quantity.

Note:

Any definition of a unit for a number, does not require an associated quantity other than 1.

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? **NO**

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

Name and definition should go hand-in-hand. Amount is a term with a far too general meaning in common English language to be "monopolized" for metrology.

Amount is not a property of a substance and is therefore not covered by the VIM definition of quantity.

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

The quantity amount of substance is to be renamed. IUPAC requested a new name for amount of substance in 2009 from CCQM and CCU in 2009. That request should be available before IUPAC draws conclusions on its understanding of the concept amount of substance which must

take into account that the unit 1 is a natural unit for numbers, and the mole -a natural multiple of 1- a natural unit for a specified large number.

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Names such as number of entities, numerousness, numerosity, are possibilities.

Date: Oct. 1, 2014

Prof. Dr. Jürgen Stohner

Chairman of the Task Group "A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities"

Dear Professor Stohner,

Thanks a lot for your letter dated June 1, 2014. As response to your mail, please find below the answers to the questionnaire.

1. Are you (as NAO representing your members) satisfied with the current definition of the mole?
a. YES or NO? **Answer: YES**
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? **Answer: YES**
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? **Answer: YES**
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? **Answer: YES**
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.

Thanking you,

Yours sincerely,

Dr. Rameshwar Adhikari

President

Nepal Polymer Institute (NPI); Post Box 24411, Kathmandu, NEPAL E-mail: nepalpolymer@gmail.com Webpage: www.nepalpolymer.org

United Kingdom

Tue, 20 Jan 2015 01:42:42 -0800 (PST)
From: David Clark <clarkd@rsc.org>
To: "mole@iupac.org" <mole@iupac.org>
CC: "cjhumphris@btinternet.com" <cjhumphris@btinternet.com>,
"g.p.moss@qmul.ac.uk" <g.p.moss@qmul.ac.uk>
Subject: UK Response to the Proposed Definition of the Mole.
Thread-Topic: UK Response to the Proposed Definition of the Mole.

Dear Sir or Madam,

I write as secretary to the RSC's IUPAC Committee and also to the RSC's Committee on Standards and Nomenclature. We have discussed the proposed definition of the mole within both committees and as an NAO, we accept the new definition, although with some reservations (see attached response from one of the committee members). We are also working with Prof. Ian Mills, the former President of the Consultative Committee for Units (CCU) who has been closely involved with the redefinition project for a number of years.

Another issue that has been raised with the committees is the need for clear documentation and guidance, for teachers at university and school level, on how to teach the new concept of the mole.

Kind Regards

David Clark

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Head of Emerging Markets
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Mole is the name of the SI base unit (symbol mol) for the base quantity amount of substance (symbol n) which is defined in IUPAC documents (e.g. IUPAC Green Book, 3rd Edition, 2nd Printing 2008 [4]) using the expression $n = N/N_A$, where N is the number of entities, and N_A is the Avogadro constant. Similarly, the SI Brochure (8th Edition 2006 [2]) provides the following definition of the quantity amount of substance:

"Amount of substance is defined to be proportional to the number of specified elementary entities in a sample, the proportionality constant being a universal constant which is the same for all samples … This constant is called the Avogadro constant, symbol N_A or L … the relation is $n = N/N_A$. … the Avogadro constant has the coherent SI unit reciprocal mole."

QUESTIONNAIRE

IUPAC NAOs are hereby asked the following: I write as NR of IUPAC Division IV but do not necessarily express the view of other Division IV members.

1. Are you (as NAO representing your members) satisfied with the current definition of the mole?

a. YES or NO? NO

b. If NO, please specify in a few sentences why you opted for NO. Because it does not convey the essence of there being the same number of elemental entities in a mole regardless of the substance under consideration.

c. If NO, please provide some suggestion on what to change. Adopt the new definition.

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? YES

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? YES

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? YES

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.

2/3Because of external time-constraints, Chemical Societies represented by IUPAC NAOs are asked to reply no later than 2014/October/01. The replies should be drafted on a letterhead, signed, and sent in as a PDF format to mole@iupac.org. The comments will be used towards formulating the IUPAC Technical Report. Those organizations who will reply will be sent an advance draft of the IUPAC Technical Report for further comment and input before submission to Pure and Applied Chemistry.