Committee on
Nomenclature Terminology, and Symbols

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)