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IUPAC Recommendations

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Definition of the mole (IUPAC Recommendation 2017)

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Abstract: In 2011 the General Conference on Weights and Measures (CGPM) noted the intention of the International Committee for Weights and Measures (CIPM) to revise the entire International System of Units (SI) by linking all seven base units to seven fundamental physical constants. Of particular interest to chemists, new definitions for the kilogram and the mole have been proposed. A recent IUPAC Technical Report discussed these new definitions in relation to immediate consequences for the chemical community. This IUPAC Recommendation on the preferred definition of the mole follows from this Technical Report. It supports a definition of the mole based on a specified number of elementary entities, in contrast to the present 1971 definition.

Keywords: Avogadro constant; Avogadro number; definition; IUPAC Physical and Biophysical Chemistry Division; mole; SI.

1 Introduction

The 9th General Conference on Weights and Measures (CGPM) instructed the International Committee for Weights and Measures (CIPM) in 1948 "to make recommendations for a single practical system of units of measurement, suitable for adoption by all countries adhering to the Metre Convention" [1]. In 1954, the 10th CGPM adopted a practical system of units of measurements for international use. It contained six base units: the metre, kilogram, second, ampere, degree Kelvin (later renamed kelvin), and candela [2]. This international system was named "Système International d'Unités" (engl. International System of Units) and abbreviated as SI by the 11th CGPM [3]. The seventh base unit, the mole, was added to the SI in 1971 by the 14th CGPM [4].

The International Bureau of Weights and Measures (BIPM) publishes the SI Brochure with the intent "to define and promote the SI, which has been used around the world as the preferred language of science and

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technology since its adoption in 1948" [5]. The SI is an evolving system that reflects current best measurement practices. Thus, changing the definition of base units of measurement is not an unprecedented or unusual action. The evolving definition of the metre is an example of this. Early adoption of the metre as the unit of length by the French government resulted in its definition as the 1:10 000 000 part of the meridian through Paris between the North Pole and the equator. A century later, the first meeting of the CGPM in 1889 sanctioned a new platinum-iridium prototype metre bar, which served as the official international metre until 1960. The desire to adopt an indestructible standard and advances in interferometry led the 11th CGPM to further redefine the metre as "the length equal to 1 650 763.73 wavelengths in vacuum of the radiation corresponding to the transition between the levels $2p_{10}$ and $5d_5$ of the krypton 86 atom" in 1960 [6] (we note that IUPAC recommends writing "krypton-86" [7]). Fixing the velocity of light to a constant value, the metre was last redefined by the 17th CGPM in 1983 as "the length of the path travelled by light in vacuum during a time interval of 1/299 792 458 of a second" [8].

The present SI has several important shortcomings (see [9] and references therein). Notably, the base unit kilogram is based on an artifact, a platinum-iridium cylinder (the international prototype kilogram, IPK) manufactured in 1879 and stored at the BIPM. There is an intrinsic uncertainty in the long-term stability of the IPK. In principle, this instability also impacts other SI units that depend on the kilogram, among which is the mole.

In 1999, the 21st CGPM recommended that "national laboratories continue their efforts to refine experiments that link the unit of mass to fundamental or atomic constants with a view to a future redefinition of the kilogram" [10]. Furthermore, in 2011 the CGPM noted the intention of the CIPM to revise the entire SI by linking all seven base units to seven constants [11, 12].

In a recent IUPAC Technical Report [9], a thorough analysis of the discussion on the impact of the proposed new definitions of two key units for chemists was undertaken: the kilogram and the mole. The present recommendation focuses on the unit mole. In Section 2 a brief summary of the discussion is recalled, in Section 3 the recommended definition of the mole is formulated, and in Section 4 some additional remarks and explanations are presented.

2 Discussion

The proposal for the new definition of the mole initiated a lively debate between chemists who preferred the change and others who thought it better to retain an explicit link to the mass of carbon-12.

The amount of chemical substances is traditionally measured by mass or volume. Since the introduction of relative atomic masses (also called "atomic weights") by John Dalton (see for example [13]), chemists are able to express their observations in a quantity that is proportional to the number of elementary entities (see below) [4]. The unit of the SI quantity "amount of substance" in its present definition still relies on the mass of the international prototype kilogram [4]:

1. "The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kg 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."

We note that IUPAC recommends writing "carbon-12" [7]. Thus, the 1971 definition refers to well-defined number of atoms in a certain fixed mass of carbon-12. With the recent advances in science and measurement practice, our ability to determine the value of the Avogadro constant has now reached a level of relative uncertainty that allows a redefinition of the mole in terms of the explicit number of elementary entities. While this conceptual change does not bring any immediate practical benefits to our ability to better realize the mole, it realigns the definition of the mole with the way most chemists understand it [9].

3 Definition of the mole

> The mole, symbol mol, is the SI unit of amount of substance. One mole contains exactly 6.022 140 76 × 10^{23} elementary entities. This number is the fixed numerical value of the Avogadro constant, N_A, when expressed in mol^{-1}, and is called the Avogadro number.
> The amount of substance, symbol n, of a system 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 amount of B, n(B), is proportional to the number of entities of B, N(B), with

$$n(\mathrm{B}) = N_\mathrm{A}^{-1}\, N(\mathrm{B}) \tag{1}$$

The proportionality factor is a universal physical constant that is independent of the nature of the substance. The reciprocal of the proportionality factor, N_A, is the Avogadro constant, which is the same for all substances. The stipulated Avogadro number is the fixed numerical value of the Avogadro constant, $N_A = 6.022\,140\,76 \times 10^{23}\ \mathrm{mol}^{-1}$, which is provided by the CODATA Task Group on Fundamental Constants [14].

The Avogadro constant has the SI unit mol^{-1} because amount of substance, n, is a base quantity with the SI unit mole and because the number of entities, being a number, is a quantity of dimension one. The amount of B, n(B), is also proportional to the mass of B, m(B), with

$$n(\mathrm{B}) = M(\mathrm{B})^{-1}\, m(\mathrm{B}) \tag{2}$$

The proportionality factor is the reciprocal of the molar mass, M(B), which is a characteristic constant of the substance B.

4 Explanatory remarks

A better understanding of the above definition requires some explanation and guidance. Below are some remarks that might help the reader to gain a better understanding of the above definition.

1. Although the full name of the quantity is the amount of substance, the word “substance” is a placeholder and should be replaced with the name of the actual substance concerned. Thus, for example, one speaks of the “amount of water”, $n(H_2O)$, rather than “amount of substance of water”.
2. The name “amount of substance” is not universally considered a good choice [15] and this quantity is sometimes also called “chemical amount” [9, 16]. A thorough examination of a potential alternative name for the quantity amount of substance, n, has to be performed.
3. The 1971 definition of the mole implies that the Avogadro number equals the ratio of the gram to the dalton ($m_u = 1\ \mathrm{u} = 1\ \mathrm{Da}$), with the value of the dalton (Da) expressed in gram. The historical continuity of the present definition preserves this relation, not exactly, but to within an uncertainty negligible for practical purposes.
4. The 1971 definition of the mole is understood to apply to an ensemble of unbound atoms at rest and in their ground state. While these requirements are often ignored, the new definition of the mole decouples the mole from the kilogram and therefore the condition that the atoms must be in the unbound state is no longer required. Thus, one can say that 0.012 kg of pure carbon-12 in the form of graphite is not *exactly* 1 mol under the 1971 definition of the mole if the carbon is in solid form, and at room temperature. The relative error that is incurred, which is rarely corrected, is negligible, but similar in magnitude to the relative uncertainty of the molar mass constant under the new definition of the mole.
5. The word “system” in the 1971 definition of the mole (see Section 2) refers to the group of specified entities. The system should be evident from this specification and need not be mentioned here.
6. The definition of the mole which appears in Section 3 was agreed upon at the 23rd meeting of the Consultative Committee for Units (CCU) in September 2017. Afterwards, the CIPM decided to submit this definition to the 26th CGPM which meets in November 2018 [17].

7. The definition of the mole which appears in Section 3 deviates slightly from the original text proposed in the IUPAC Technical Report [9] (see also Remarks 2 and 5).

The molar mass of any entity B, M(B), may still be obtained from its relative atomic mass (also called "atomic weight"), A_r(B), from the equation

$$M(\mathrm{B}) = A_\mathrm{r}(\mathrm{B})M(^{12}\mathrm{C})/12 = A_\mathrm{r}(\mathrm{B})M_\mathrm{u} \tag{3}$$

where M_u is the molar mass constant, equal to $M(^{12}\mathrm{C})/12$. Because the molar mass of unbound carbon-12, $M(^{12}\mathrm{C})$, is no longer 12 g mol^{-1} exactly, the molar mass constant, M_u, is no longer 1 g mol^{-1} exactly. The uncertainty of M_u, being smaller than 1 part in 10^9, however, is of no practical relevance for chemistry (see the discussion following eq. 16 and Section 5.3 in [9]). Within this uncertainty, the value of M_u remains 1 g mol^{-1}. The molar mass of any entity B, M(B), is also related to the mass of the elementary entity, m_a(B), by the equation

$$M(\mathrm{B}) = N_\mathrm{A}\, m_\mathrm{a}(\mathrm{B}) = N_\mathrm{A}\, A_\mathrm{r}(\mathrm{B})m_\mathrm{u} \tag{4}$$

where m_u is the atomic mass constant equal to the atomic mass of carbon-12 divided by 12, $m_a(^{12}\mathrm{C})/12$. Both M_u and m_u are related to the Avogadro constant through the equation $M_u = N_A m_u$.

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