

IUPAC Recommendations

Roberto Marquardt, Juris Meija, Zoltán Mester, Marcy Towns, Ron Weir, Richard Davis and Jürgen Stohner*

Definition of the mole (IUPAC Recommendation 2017)

<https://doi.org/10.1515/pac-2017-0106>

Received January 11, 2017; accepted September 12, 2017

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

Article note: Sponsoring bodies: IUPAC Physical and Biophysical Chemistry Division, IUPAC Inorganic Chemistry Division, IUPAC Analytical Chemistry Division, IUPAC Committee on Chemistry Education, and IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols: see more details on page 178.

***Corresponding author: Jürgen Stohner**, ZHAW Zürich University of Applied Sciences, ICBT Institute for Chemistry and Biotechnology, Einsiedlerstrasse 31, CH 8820 Wädenswil, Switzerland, e-mail: sthj@zhaw.ch; and Guest scientist at: ETHZ Swiss Federal Institute of Technology, Laboratory for Physical Chemistry, ETH Hönggerberg, Wolfgang-Pauli-Strasse 10, CH-8092 Zürich, Switzerland, e-mail: just@phys.chem.ethz.ch

Roberto Marquardt: Laboratoire de Chimie Quantique, Institut de Chimie, Université de Strasbourg, 1 Rue Blaise Pascal, F-67008 Strasbourg, France

Juris Meija and Zoltán Mester: National Research Council Canada, Measurement Science and Standards, 1200 Montreal Road M-12, Ottawa, ON K1A 0R6, Canada

Marcy Towns: Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN, USA

Ron Weir: Department of Chemistry and Chemical Engineering, Royal Military College of Canada, P.O. Box 17000, Stn. Forces, Kingston, ON K7K 7B4, Canada

Richard Davis: Bureau International des Poids et Mesures, Pavillon de Breteuil F-92312, Sèvres Cedex, France

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 $6.022\,140\,76 \times 10^{23}$ 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, $n(\text{B})$, is proportional to the number of entities of B, $N(\text{B})$, with

$$n(\text{B}) = N_A^{-1} N(\text{B}) \quad (1)$$

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, $N_A = 6.022\,140\,76 \times 10^{23} \text{ mol}^{-1}$, 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, $n(\text{B})$, is also proportional to the mass of B, $m(\text{B})$, with

$$n(\text{B}) = M(\text{B})^{-1} m(\text{B}) \quad (2)$$

The proportionality factor is the reciprocal of the molar mass, $M(\text{B})$, 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”, $n(\text{H}_2\text{O})$, 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 ($m_u = 1 \text{ u} = 1 \text{ Da}$), 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

$$M(B) = A_r(B)M(^{12}\text{C})/12 = A_r(B)M_u \quad (3)$$

where M_u is the molar mass constant, equal to $M(^{12}\text{C})/12$. Because the molar mass of unbound carbon-12, $M(^{12}\text{C})$, 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 10⁹, 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

$$M(B) = N_A m_a(B) = N_A A_r(B) m_u \quad (4)$$

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

5 Membership of sponsoring bodies

Membership of the IUPAC Physical and Biophysical Chemistry Division for the period 2014–2015 was as follows:

President: R. Marquardt (France); **Secretary:** A. Friedler (Israel); **Vice President:** A. K. Wilson (USA); **Past President:** K. Yamanouchi (Japan); **Titular Members:** K. Bartik (Belgium); A. R. Goodwin (USA); A. E. Russell (UK); J. Stohner (Switzerland); Y. H. Taufiq-Yap (Malaysia); F. van Veggel (Canada); **Associate Members:** A. Császár (Hungary); V. Yu. Kukushkin (Russia); A. W. Mombrú Rodríguez (Uruguay); X. S. Zhao (China); K. Bhattacharyya (India); J. L. B. M. de Faria (Portugal); **National Representatives:** J. Cejka (Czech Republic); S. Hannongbua (Thailand); M. Koper (The Netherlands); J. E. G. Mdoe (Tanzania); V. Tomišić (Croatia); A. bin Hasan Susan (Bangladesh); S.-J. Kim (South Korea); E. Klein (Bulgaria); M. Korenko (Slovakia); K. E. Laasonen (Finland); H. Corti (Argentina).

Membership of the IUPAC Inorganic Chemistry Division for the period 2014–2015 was as follows:

President: J. Reedijk (Netherlands); **Secretary:** M. Leskelä (Finland); **Vice President:** L. R. Öhrström (Sweden); **Past President:** R. D. Loss (Australia); **Titular Members:** T. Ding (China); M. Drábik (Slovakia); D. Rabinovich (USA); E. Tshuva (Israel); T. Walczyk (Singapore); M. Wieser (Canada); **Associate Members:** J. Buchweishaija (Tanzania); J. García-Martínez (Spain); P. Karen (Norway); A. Kiliç (Turkey); K. Sakai (Japan); R.N. Vannier (France); **National Representatives:** Y. Abdul Aziz (Malaysia); L. Armelao (Italy); A. Badshah (Pakistan); V. Chandrasekhar (India); J. Galamba Correia (Portugal); S. Kalmykov (Russia); S. Mathur (Germany); L. Meesuk (Thailand); B. Prugovečki (Croatia); N. Trendafilova (Bulgaria).

Membership of the IUPAC Analytical Chemistry Division for the period 2014–2015 was as follows:

President: D. Brynn Hibbert (Australia); **Secretary:** Z. Mester (Canada); **Vice President:** J. Labuda (Slovakia); **Past President:** M. Filomena Camões (Portugal); **Titular Members:** C. Balarew (Bulgaria); Y. Chen (China); A. Felinger (Hungary); H. Kim (South Korea); C. Magalhães (Portugal); H. M. M. Sirén (Finland); **Associate Members:** R. Apak (Turkey); P. Bode (The Netherlands); D. Craston (UK); Y. Heng Lee (Malaysia); T. Maryutina (Russia); N. Torto (South Africa); **National Representatives:** P. DeBièvre (Belgium); M. N. Eberlin (Brazil); P. Novak (Croatia); L. Charles (France); D. Mandler (Israel); J. Hanif (Pakistan); A. Fajgelj (Slovenia); O. Chande Othman (Tanzania); K. Grudpan (Thailand); D. G. Shaw (USA).

Membership of the IUPAC Committee on Chemistry Education for the period 2014–2015 was as follows:

President: M.-H. Chiu (China); **Secretary:** J. Apotheker (The Netherlands); **Titular Members:** N. H. K. Aremo (Finland); S. Boniface (New Zealand); M. Kamata (Japan); R. M. Naaman (Israel); M. Sözbilir (Turkey); M. Towns (USA); **National Representatives:** A. H. Wright (Australia); M. M. Rahman (Bangladesh); L. Brandt (Belgium); B. Toshev (Bulgaria); L. L. Santibañez (Chile); Z. Shuai (China); T. Solomon (Ethiopia); C. S. Reiners (Germany); M. Riedel (Hungary); U. Maitra (India); P. E. Childs (Ireland); L. Cardellini (Italy); A. A. Al-Najjar (Kuwait); T.-K. Soon (Malaysia); R. Adhikari (Nepal); F. Mahmood (Pakistan); A. Pokrovsky (Russia); M. Elmgren (Sweden); P. Boesch (Switzerland); S. Tantayanon (Thailand); M. Z. Hoffman (USA); T. Overton (UK); **Division Representatives:** A. Russell (UK); J. García-Martínez (Spain); M. J. Garson (Australia); W. Mormann (Germany); Y. Chen (China); M. Dassenakis (Greece); J. H. Duffus (UK); R. M. Hartshorn (New Zealand).

Membership of the IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols for the period 2014–2015 was as follows: **Chair:** R. Weir (Canada); **Secretary:** J. Stohner (Switzerland); **Titular Members:** J. Frey (UK); J. Meija (Canada); G. P. Moss (UK); **Associate Members:** R. Cornelis (Belgium); M. Drábik (Slovakia); J. Kaiser (UK); **Division Representatives:** M. Drábik (Slovakia); M. Brimble (New Zealand); P. S. Fedotov (Russia); A. Goodwin (USA); D. B. Hibbert (Australia); Y. Martin (USA); G. Moad (Australia); A. Rauter (Portugal); **Representatives of Other Organizations:** A. Authier (France) and C. Brock (USA), *International Union of Crystallography*; I. Elmadfa (Austria), *International Union of Nutritional Sciences*; S. N. Lea (UK), *International Union of Pure and Applied Physics*; D. Schomburg (Germany), *International Union of Biochemistry and Molecular Biology*; M. Spedding (France), *International Union of Pharmacology*; R. Wielgosz (France), *Bureau International des Poids et Mesures*.

Acknowledgments: This manuscript (PAC-REC-17-01-06) was prepared in the framework of IUPAC project 2013-048-1-100.

References

- [1] CGPM. *Comptes Rendus de la neuvième Conférence Générale des Poids et Mesures (1948). Résolution 6*, BIPM, URL [http://www.bipm.org/en/CGPM/db/9/6/\(1949\)](http://www.bipm.org/en/CGPM/db/9/6/(1949)).
- [2] CGPM. *Comptes Rendus des séances de la dixième Conférence Générale des Poids et Mesures (1954). Résolution 6*, BIPM, URL [http://www.bipm.org/en/CGPM/db/10/6/\(1955\)](http://www.bipm.org/en/CGPM/db/10/6/(1955)).
- [3] CGPM. *Comptes Rendus des séances de la onzième Conférence Générale des Poids et Mesures (1960). Résolution 12*, BIPM, URL [http://www.bipm.org/en/CGPM/db/11/12/\(1961\)](http://www.bipm.org/en/CGPM/db/11/12/(1961)).
- [4] CGPM. *Comptes Rendus des séances de la quatorzième Conférence Générale des Poids et Mesures (1971). Résolution 3*, BIPM, URL [http://www.bipm.org/en/CGPM/db/14/3/\(1972\)](http://www.bipm.org/en/CGPM/db/14/3/(1972)).
- [5] BIPM. *Le Système international d'unités/The International System of Units (Brochure sur le SI/SI brochure)*, 2006, BIPM, 8 edition (2006).
- [6] CGPM. *Comptes Rendus des séances de la onzième Conférence Générale des Poids et Mesures (1960). Résolution 6*, BIPM, URL [http://www.bipm.org/en/CGPM/db/11/6/\(1961\)](http://www.bipm.org/en/CGPM/db/11/6/(1961)).
- [7] N. G. Connelly, T. Dambus, R. M. Hartshorn, A. T. Hutton. *Nomenclature of Inorganic Chemistry (IUPAC Recommendations 2005)*, IUPAC and Royal Society of Chemistry, Cambridge (2005).
- [8] CGPM. *Comptes Rendus des séances de la 17e Conférence Générale des Poids et Mesures (1983). Résolution 1*, BIPM, URL [http://www.bipm.org/en/CGPM/db/17/1/\(1984\)](http://www.bipm.org/en/CGPM/db/17/1/(1984)).
- [9] R. Marquardt, J. Meija, Z. Mester, M. Towns, R. Weir, R. Davis, J. Stohner. *Pure Appl. Chem.* **89**, 951 (2017).
- [10] CGPM. *Proceedings of the 21st meeting of the General Conference on Weights and Measures (1999). Resolution 7*, BIPM, URL [http://www.bipm.org/en/CGPM/db/21/7/\(2001\)](http://www.bipm.org/en/CGPM/db/21/7/(2001)).
- [11] CGPM. *Proceedings of the 24th meeting of the General Conference on Weights and Measures (2011). Resolution 1*, BIPM, URL [http://www.bipm.org/en/CGPM/db/24/1/\(2013\)](http://www.bipm.org/en/CGPM/db/24/1/(2013)).
- [12] CGPM. *Proceedings of the 25th meeting of the General Conference on Weights and Measures (2014). Resolution 1*, BIPM, URL [http://www.bipm.org/en/CGPM/db/25/1/\(2015\)](http://www.bipm.org/en/CGPM/db/25/1/(2015)).
- [13] B. W. Petley. *IEEE Trans. Instr. Meas.* **38**, 175 (1989).

- [14] D. B. Newell, F. Cabiati, J. Fischer, K. Fujii, S. G. Karshenboim, H. S. Margolis, E. de Mirandes, P. J. Mohr, F. Nez, K. Pachucki, T. J. Quinn, B. N. Taylor, M. Wang, B. Wood, Z. Zhang. "The CODATA 2017 Values of h , e , k , and N_A for the Revision of the SI," *Metrologia*, accepted, online 20 Oct 2017, <https://doi.org/10.1088/1681-7575/aa950a> (2017).
- [15] J. Lorimer. *Chem. Int.* **32**(1), 6 (2010).
- [16] E. R. Cohen, T. Cvitaš, J. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. J. Thor. *Quantities, Units and Symbols in Physical Chemistry*, 3rd ed. IUPAC & The Royal Society of Chemistry, 3rd printing, Cambridge (2011).
- [17] CIPM. *Decision CIPM/106-10*, BIPM, URL <http://www.bipm.org/en/committees/cipm/meeting/106.html> (2017).