

CCQM Update

Richard Brown
on behalf of

Sang-Ryoul Park, CCQM President

Ad-hoc WG on the mole

- WG of the CCQM with the remit:
 - draft a "*mise en pratique*" for the realization of the mole
 - response to the CCU draft of the 9th SI Brochure
 - engagement with IUPAC activities
 - discuss and draft a new definition of the mole considering the opinions of the relevant stakeholders
 - create awareness of redefinition of the mole
- Membership: BIPM, INRIM, KRISS, NMIA, NIM, METAS, NIST, NMIJ, NPL, NRC, LGC, PTB
- 7 meetings and 2 workshops since 2010



Drafting the definition: Interaction with IUPAC

- Key stakeholder group – understanding of and teaching the mole
- Strong cooperation between CCQM & IUPAC – involvement in workshops
- IUPAC project on ‘definition of the mole’
- Draft CCQM definition of the mole was modified according to IUPAC’s comments
- Approved by the CCQM in April 2018
- Chemical community see explicit reference to N_A as a great improvement

DE GRUYTER Pure Appl. Chem. 2018; 90(3): 375–380

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.

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New definition

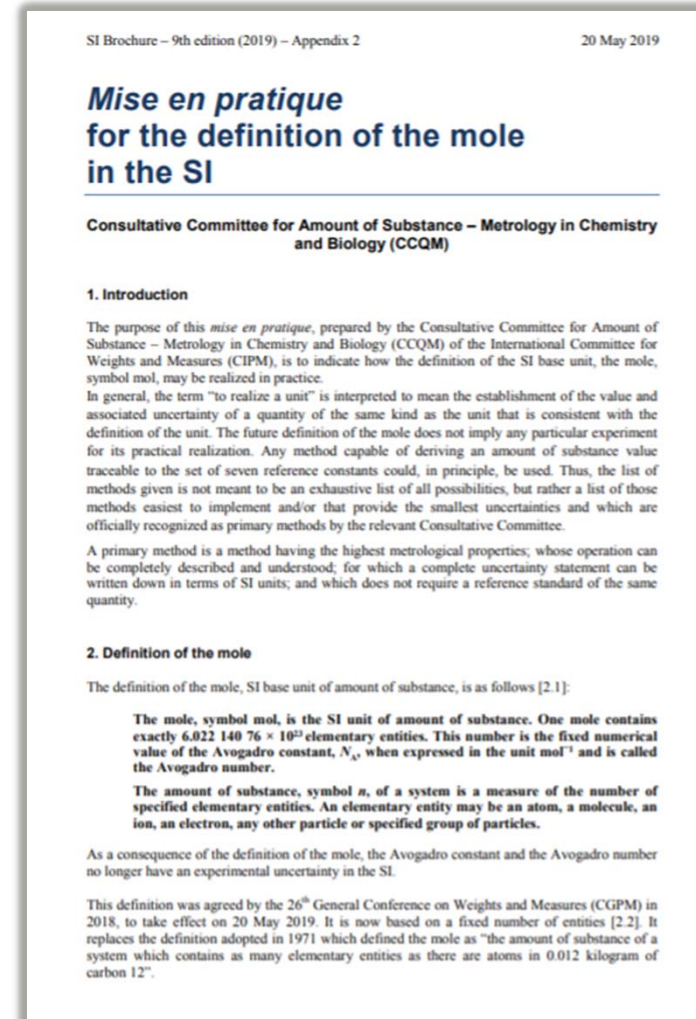
The mole

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 the unit 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.

Mise-en-pratique

- Next task was to edit the *mise-en-pratique*, in particular:
 - incorporation of the Avogadro experiment
 - coordination with CCM: mise-en-pratique of the kg
 - continuity with the existing mise-en-pratique
 - small numbers of entities
 - continuity with previous definition, u/c acquired by M_u
- Approved at the April 2019 CCQM meeting with minor comments dealt with at the start of May 2019



Dissemination of the new definition

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Amount of substance and the mole in the SI

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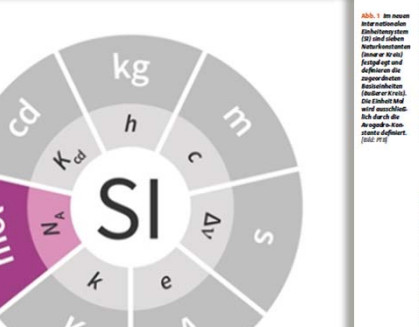
Abstract
Following the revision of the International System of Units (SI), that takes effect on 20 May 2019, the unit mole is defined by using a fixed number of elementary entities. This number is the fixed numerical value of the Avogadro constant, which is the defining constant of the unit mole. This definition was made possible because the determination of the Avogadro constant had reached a level of relative uncertainty that allowed it to be fixed and, at the same time, safeguard continuity of measurement results before and after the definition. The motivation for the revision of the SI and the mole in particular will be explained and the experimental work that allowed it is summarized.

Keywords: mole, amount of substance, Avogadro constant, Avogadro project, International System of Units, silicon
(Some figures may appear in colour only in the online journal)

1. Introduction
The definitions of the SI base units undergo a fundamental revision in May 2019 that puts the emphasis on the 'defining constants'. From the fixed numerical values of these defining constants, expressed in the units of the SI, the complete system of units can be derived. The revised definitions are based on these constants and are therefore inherently stable.
On this occasion, the definition of the mole, a centimetre of measurement in chemistry, is also revised. This required extremely accurate measurements of the relevant defining constant, the Avogadro constant, in order to assure the continuity of measurement results before and after the revision. The revised definition of the mole is as follows [1]:

'The mole, symbol mol, is the SI unit of amount of substance. One mole contains exactly 6.022 140 76 × 10²³ elementary entities. This number is the value of the Avogadro constant, N_A, fixed by definition, and is called the Avogadro constant. The amount of substance, symbol n, of a system is the quotient of the amount of elementary entities in the system and the Avogadro constant, and is expressed in moles. An elementary entity may be an atom, an electron, any other particle or of particles.'

The revised definition of the mole is the number of elementary entities (typical units) and does no longer depend on the unit of mass, the kilogram. Traceability will be established by using mass metrology, atomic masses (IUPAC), the International Applied Chemistry, using the term relative atomic mass, M_r, and the molar mass constant, M_m, relative to the carbon-12 isotope.



Analytical Methods
AMC TECHNICAL BRIEFS

Revision of the International System of Units (Background paper)

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AMC TECHNICAL BRIEFS
Revision of the International System of Units (Background paper)
Analytical Methods Committee AMCTB No 86

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The International System of Units (SI) is the only globally agreed practical system of measurement units. Stemming from the Metric Convention of 1875, which established a permanent international structure for member governments to act in common accord on all matters relating to units of measurement, the SI was revised in 1960 and is now defined by the SI Brochure. The foundation of the SI are the set of seven well defined base units: the metre, the kilogram, the second, the ampere, the kelvin, the mole, and the candela, from which all derived units (such as metres per second) can be derived. On 20 November 2018, the 26th General Conference on Weights and Measures (CGPM) adopted a new definition of the SI base units, which will take effect on 20 May 2019. The revision of the SI is the result of a long process of international cooperation and discussion, which was initiated in 1993 with the adoption of the SI Brochure. The revision of the SI is the result of a long process of international cooperation and discussion, which was initiated in 1993 with the adoption of the SI Brochure.

The current international system of units (SI) and the need for change
The current international system of units (SI) is the only globally agreed practical system of measurement units. Stemming from the Metric Convention of 1875, which established a permanent international structure for member governments to act in common accord on all matters relating to units of measurement, the SI was revised in 1960 and is now defined by the SI Brochure. The foundation of the SI are the set of seven well defined base units: the metre, the kilogram, the second, the ampere, the kelvin, the mole, and the candela, from which all derived units (such as metres per second) can be derived. On 20 November 2018, the 26th General Conference on Weights and Measures (CGPM) adopted a new definition of the SI base units, which will take effect on 20 May 2019. The revision of the SI is the result of a long process of international cooperation and discussion, which was initiated in 1993 with the adoption of the SI Brochure.

Eine neu definierte SI-Einheit für die Chemie Wie viele Moleküle enthält ein Mol?

Rainer Stöckh¹, Olaf Rientz², Axel Pramann³ & Bernd Güttler⁴

Der Paradigmenwechsel für das internationale Einheitensystem (SI) wurde am 20. Mai 2019 vollzogen. Von diesem Tag an sind alle sieben Basis-Einheiten im internationalen Einheitensystem mit Hilfe festgelegter Naturkonstanten definiert. Dies gilt auch für das Mol, die Basis-Einheit der Stoffmenge. Was sie bisher noch von der Definition des Kilogramms abhängig, so wird sie im neuen SI allein durch die Avogadro-Konstante definiert. Eine weitreichende Konsequenz ist: Schul- und Lehrbücher müssen umgeschrieben werden. Aber welche Auswirkungen hat die Neudefinition auf die metrologische Rückführung chemischer Messungen und was sind die Folgen für die Resultate chemischer Messungen im alltäglichen Leben? Anders sich etwa die Grenzwerte für Schadstoffe in der Umwelt oder in Lebensmittel? Dieser Artikel gibt einen Überblick über die alte und neue Definition der Einheit Mol und beschreibt die Auswirkungen auf chemische Messungen in der Praxis.



Es ist ein Anzeichen der Revision der Metrokonvention bis Juni 2019, dass die 26. Tagung der Generalkonferenz für Maß und Gewicht (CGPM) in Paris im November 2018 eine grundlegende Revision des internationalen Einheitensystems (SI) beschlossen hat. In diesem Fall wird das Mol, die Einheit der Stoffmenge, von der Definition des Kilogramms unabhängig, so wird sie im neuen SI allein durch die Avogadro-Konstante definiert. Eine weitreichende Konsequenz ist: Schul- und Lehrbücher müssen umgeschrieben werden. Aber welche Auswirkungen hat die Neudefinition auf die metrologische Rückführung chemischer Messungen und was sind die Folgen für die Resultate chemischer Messungen im alltäglichen Leben? Anders sich etwa die Grenzwerte für Schadstoffe in der Umwelt oder in Lebensmittel? Dieser Artikel gibt einen Überblick über die alte und neue Definition der Einheit Mol und beschreibt die Auswirkungen auf chemische Messungen in der Praxis.

ASPECTE
BIOCHIMICAL SCIENCES 21, 2019, 610-612

MOL UND AVOGADRO-KONSTANTE

Bernd Güttler, Peter Becker, Horst Bettin, Axel Pramann, Olaf Rientz

1. EINLEITUNG
Für die Einheit Mol und Kilogramm, aber auch Ampere und Kelvin werden am 20. Mai 2019 durch die Generalkonferenz für Maß und Gewicht der Metrokonvention neue Definitionen eingeführt. Die neuen Definitionen sind durch die Festlegung von bestimmten Naturkonstanten definiert, die durch die Festlegung von bestimmten Naturkonstanten definiert sind. Die neuen Definitionen sind durch die Festlegung von bestimmten Naturkonstanten definiert, die durch die Festlegung von bestimmten Naturkonstanten definiert sind.

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.
Die molekulare Überlegung in der europäischen Richtlinie 90/269/EWG lautet:
Das Mol, Einheit der Stoffmenge, ist die Einheit der Stoffmenge. Ein Mol enthält genau 6,022 140 76 × 10²³ Elementarteilchen. Diese Zahl entspricht dem für die Avogadro-Konstante N_A genannten Zahlenwert, ausgedrückt in der Einheit mol⁻¹, und wird als Avogadro-Zahl bezeichnet.
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The Avogadro Constant for the Definition and Realization of the Mole
Bernd Güttler¹, Olaf Rientz², and Axel Pramann³

The International System of Units (SI) base unit of the quantity 'amount of substance' is the mole (symbol: mol). After the revision of the SI to be implemented in 2019, when all SI units will be based solely on constants, the mole will be defined through a fixed value of the Avogadro constant N_A. One mole contains exactly 6.022 140 76 × 10²³ elementary entities, meaning the mole will no longer be linked to the kilogram. Currently, the mole is defined via the mass of exactly 0.012 kg of the ¹²C isotope which links it to the kilogram prototype. The history, changes, and implications of the revised definition of the mole are discussed here from the chemist's point of view. The ability to count entities such as atoms or molecules precisely enough to enable a revision of the SI and preserve consistency of previous and future measurements is crucial. This is achieved with the realization of the Avogadro constant based on the ²⁸Si crystal density (CCD) method (counting the atoms in a silicon sphere). The determination of N_A, focusing on the measurement of the molar mass of silicon highly enriched in the ²⁸Si isotope, with the lowest uncertainty so far is presented.

The mole is the amount of substance of a system that contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12. Here, the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, or other particles, or specified groups of such particles.
This definition clearly demonstrates the relation of the mass of an entity and its amount of substance. The mole is one out of a set of seven base units of the SI. Although the mole and the kilogram are defined as independent base units, they are closely related to each other. In the 1971 definition, one mole of ¹²C has a mass of exactly 12 g. This in turn means that the instrument to determine the mass of an object – a balance – is also used to determine the amount of substance. In every chemical case a unit balance is used to measure the mass of a substance, yielding it to be the respective molar mass M (unit g mol⁻¹), finally yielding the amount of substance n (unit mol) by dividing the mass m by the molar mass M. Here, the amount of substance is needed for applying the principles of quantitative chemistry and stoichiometry. If it is known that a certain amount of substance of an object will react to a certain amount of substance of a product, the chemist can calculate the respective masses and can use balance or – if the densities are known – volumetric methods, to prepare the correct amounts for that reaction. This in turn means that the amount of substance differs from the mass in particular by the fact that identical amount of substances of different materials contain the same number of atoms, molecules, or other particles, but usually do not have the same mass.
The revised definition of the mole is as follows:
'The mole, symbol mol, is the SI unit of amount of substance. One mole contains exactly 6.022 140 76 × 10²³ elementary entities. This number is the fixed numerical value of the Avogadro constant, N_A, when expressed in the unit mol⁻¹ and is called the Avogadro constant.'
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.
In other words, one mole of a substance contains exactly 6.022 140 76 × 10²³ specified entities. The above definition of the mole includes already a fixed value of the Avogadro constant

1. Introduction
The scientific community is close to a paradigm change: the planned revision of the International System of Units (SI) is already based on exact and fixed fundamental constants without the need of bringing any artifact. After the 26th meeting of the General Conference on Weights and Measures (CGPM) the need of a revised definition of the SI based on fixed fundamental constants was foreseeable and recommended by the International Committee for Weights and Measures (ICPM) in 2007.^{1,2} The revision is expected to enter into force on May 20, 2019. In the present paper, we will focus on the SI unit mole (symbol: mol). With this background, a survey of previous work related with this subject have been published. However, the authors of this review do not intend to compile a complete list of the reviewable literature and refer to the extensive references already cited in other review articles.³⁻⁵ The mole is the SI base unit that has been introduced and defined by the CGPM as follows:⁶
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.
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The IUPAC (nomenclature) for the authority of this article can be found under http://dx.doi.org/10.1039/c9ay00018a
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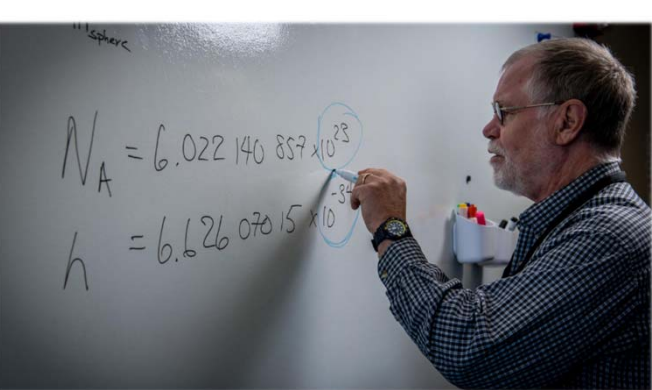
Welcome to the Update to SI Units Webinar (Slide 1 of 7)

The webinar will start shortly. All attendees are muted.

Webinar Presenters

Jeff Ruddell
Strategic Development Director - UKAS

Richard Brown
Head of Metrology - NPL



Other CCQM activities

- Traceability exceptions
 - One exception in the CIPM-MRA, for isotope ratio measurement
 - New IRWG established in CCQM, making progress with addressing these issues

- Method defined measurands
 - Defines requirements to be met for measurands to be eligible for CMC claims
 - Importantly, results expressed in SI units with metrologically valid methods are SI traceable

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TRACEABILITY EXCEPTION:

DELTA VALUE ISOTOPE RATIO MEASUREMENTS

Delta value isotope ratio measurements that cannot presently be made traceable to the SI should be made traceable to materials* recognised as International Standards. Since at present, values assigned to these materials are based on consensus values, these materials are not listed in the Appendix C of the BIPM Database.

* A list of certified reference materials that should be used to identify accepted references for delta value isotope ratio traceability statements is published and maintained by IUPAC:

Willi A. Brand, Tyler B. Coplen, Jochen Vogl, Martin Rosner and Thomas Prohaska
Assessment of international reference materials for isotope-ratio analysis (IUPAC
Technical Report)
Pure Appl. Chem. 2014, **86**(3), 425-467

The report is available for free download:
<http://www.degryter.com/doi/10.1515/pac-2013-1023>

The CIPM notes that assigned values for replacement materials should be done through a formal internationally vetted procedure that assures the continued comparability of delta value measurements.

The CIPM encourages the continuation of programmes within the NMIs to develop absolute isotope ratio measurement values for such Reference Materials and active engagement with the IUPAC community.