Definition of the mole (IUPAC Recommendation 2017)

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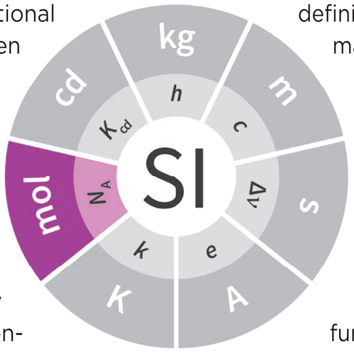
Pure and Applied Chemistry, 2018
Volume 90, Issue 1, pp. 175–180

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 (*Pure Appl. Chem.* **89**, 951 (2017); https://doi.org/10.1515/pac-2016-0808) 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 that Technical Report. It supports a definition of the mole based on a specified number of elementary entities, in contrast to the present 1971 definition.



The new definition is:

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, or any other particle or specified group of particles.

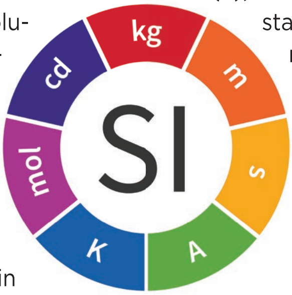
This new definition is in contrast to the current definition, adopted in 1971, which relies on the mass of the kilogram. The new definition comes in advance of the anticipated revision of SI, announced in 2011 by the General Conference on Weights and Measures of the Bureau International des Poids et Mesures (BIPM), the international body responsible for the global comparability of measurements. The new SI will link all seven base units to fundamental physical constants. In November 2018, revised definitions of the kilogram, ampere, kelvin, and mole are expected to be approved by the CGPM. The revised definitions are expected to come into force on World Metrology Day, 20 May 2019

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

On the future revision of the SI

At its 25th meeting (November 2014) the CGPM adopted a Resolution on the future revision of the International System of Units. This Resolution built on the CGPM's previous Resolution (2011), which took note of the CIPM's intention to propose a revision of the SI and set out a detailed roadmap towards the future changes.

In the revised SI four of the SI base units—namely the kilogram, the ampere, the kelvin and the mole—will be redefined in terms of constants; the new definitions will be based on fixed numerical values of the Planck constant (*h*), the elementary charge (*e*), the Boltzmann constant (k_B), and the Avogadro constant (N_A), respectively. Further, the definitions of all seven base units of the SI will also be uniformly expressed using the explicit-constant formulation, and specific mises en pratique will be drawn up to explain the realization of the definitions of each of the base units in a practical way.



https://www.bipm.org/en/measurement-units/rev-si/

Reactions/comments to the new definition of the mole

Peter W. Atkins—I have always been puzzled by the widespread view that the mole is a difficult subject. It has always seemed to me that many instructors tell their students that it is a sophisticated concept, and the students then wonder what all the fuss is about, suspecting that they have misunderstood it or have not appreciated its subtlety. The new definition cuts to the core of the meaning of 1 mole, and is therefore to be welcomed. Although there are subtleties in its determination, there can no longer be any excuse for misunderstanding its definition. How important it is, too, to distinguish the Avogadro number from the Avogadro constant.

The other aspect to be welcomed is the comment on the name 'amount of substance' with its emphasis on the word 'substance' as merely a place-holder for the entities under discussion. 'Amount of substance', it is widely accepted, is too much of a mouthful for daily use, and although they do not mention it, IUPAC is happy with the synonym 'chemical amount'. Even that, I think, is too long, and not a happy companion when the entities are photons or electrons. Happily, the authors are reluctant to proliferate new names, and I would like to think that one day the single word 'amount' will be the short, uncluttered name of what we measure in moles. We are moving towards that usage.

I suspect that the ungainly name 'amount of substance' and the widely used but regrettable colloquial expression 'number of moles' stem from the historical facts that the physical quantity is a late entry into our vocabulary (compared with mass, length, and time) and that only one unit (the mole) has ever been used to report its value. Thus, chemists have seen 'amount' and 'mole' as unambiguous synonyms and have not acquired the habit of distinguishing the fundamentally unit-free physical quantity from a specific choice of unit.

I do worry, though, about how we shall introduce the definition of the kilogram, as it changes from pointing to a lump of metal to a sophisticated definition that involves Planck's constant. I suspect that in introductory contexts we shall simply admit defeat and put in an appropriate footnote.

Peter Atkins was an Oxford professor of chemistry and fellow of Lincoln College until his retirement in 2007. He has written numerous major textbooks, including *Physical Chemistry, Inorganic Chemistry, Molecular Quantum Mechanics, Physical Chemistry for the Life Sciences,* and *Elements of Physical Chemistry.* Until 2005, he chaired the IUPAC Committee on Chemistry Education.

Bob Bucat—In terms of the basic practice of chemistry, the proposed philosophical re-definition would change nothing. Pedagogically, I believe that the teaching and learning of the concept of chemical amount, and its unit (mole), will be considerably simplified.

What a simple definition for the mole, with the number of entities specified directly: One mole contains exactly $6.022\,140\,76 \times 10^{23}$ elementary entities.

Conceptually, this is so much more easily understood than the previous mind-screwing definition, with its indirect specification of the number of entities in 1 mole: 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.

Of course, students will rightly ask, "Why this strange number?" It seems not too difficult to accept the explanation that this number is chosen for convenience: it happens to be our best estimate of the number of carbon atoms in 0.012 kilogram of carbon-12. This provides us with a standard for measuring numbers of atoms/molecules/ions by measuring mass. [Please don't let me hear a professional chemist say "But it is essentially the same thing!". Indeed, it is but I am considering this, not from the point of view of a practising chemist, so much as from the novice school students struggling to come to grips with its meaning.]

How are we supposed to remember this number? Of course, we don't need to. For example, in considering the reaction between sodium and chlorine, the important concept is that one mole of solid sodium contains the same number of atoms as the number of molecules in one mole of chlorine gas (whatever that number is). Then we can let logic take over to do stoichiometric calculations, as is the case now.

In summary, I believe that the newly proposed definition will facilitate the pedagogy relevant to these concepts.

What is a little worrisome is the proposed definition (or explanation?) of chemical amount: The chemical amount, n, is a measure of the number of specified elementary entities. That sounds very much like it is a number: how else does one measure, but with a number? But it is not a number! I understand the complexity of wording the definition of this concept, but this proposed one will perhaps (or surely, in my view) create the conception of a chemical amount as a number—a conception that will be difficult to amend.

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