

Resolving Ontological Circularity and Pedagogical Confusion Inherent in the 2019 Mole Definition by Recognizing the Elementary Amount and Adopting the Entity as the Appropriate Atomic-Scale Amount Unit

Brian Phillip Leonard

bp1eona@uakron.edu

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Abstract

The 2019 redefinition of the mole created an apparent circularity: the mole is defined in terms of the Avogadro constant N_A , but N_A is uniquely expressed in terms of the mole. And describing n as “a measure” of N has reignited the debate about whether “amount” is a legitimate physical quantity or merely a dimensionless “count”. The resulting lack of clarity exacerbates the confusion surrounding the “mole concept”. This paper proposes a resolution of both the ontological and pedagogical crises by introducing the “elementary amount” n_a —the amount of a single atomic-scale entity (of any substance)—as a constant of Nature (dimension N), analogous to the elementary charge, e . Then N_A is uniquely defined as $1/n_a$, independently of any chosen amount unit. Amount of substance is immediately recognized as an amount aggregate, $n(X) = N(X) n_a$, mirroring a mass aggregate, and the mole is defined directly as $1 \text{ mol} = N_{\text{Avo}} n_a$. The atomic-scale amount unit entity (symbol ent, dimension N), is defined as $1 \text{ ent} = n_a$, paralleling the dalton, $1 \text{ Da} = m_u$. The molar mass constant is $M_u = m_u/n_a = 1 \text{ Da/ent}$ (exactly). The selective use of ent or mol guarantees that the dimension N is retained across the entire micro-to-macro spectrum, seamlessly handling transitions between discrete and continuous regimes. This has many pedagogical advantages, especially for stoichiometry. Finally, the ontological debates about the “dimension” of amount are defused by noting that: without an underlying amount (at any scale), there would be nothing to count.

1. Introduction: confusion about the “mole concept”

1.1 The implied circularity in the 2019 definition

The SI base quantity amount of substance, its macroscopic unit, the mole, and especially the Avogadro constant are among the least well understood concepts in the STEM curriculum. The well-documented widespread confusion (Furio et al. 2002, Pekdağ et al. 2013, Leonard 2016, Moss and Pabari 2016, Rees and Bruce 2022) has recently been exacerbated by what appears to be circular logic inherent in the 2019 redefinition of the mole (Kacker and Irikura 2025a), an on-going debate about the meaning of “amount” as an independent dimension (Schmidt-Rohr 2020, Ghibaudi et al. 2024), and in particular the physical nature of the Avogadro constant (Kacker and Irikura 2025b)—collectively known as the “mole concept” (Fang et al. 2014).

The SI Brochure (BIPM 2025) states that the 2019 redefinition of the mole *implies* the following exact relation for the Avogadro constant

$$N_A = 6.022\,140\,76 \cdot 10^{23} \text{ mol}^{-1} \quad (1)$$

And this is by far the most common “definition” of the Avogadro constant found in textbooks, dictionaries, and online tutorials (Atkins et al. 2023). As explained in the SI Brochure, inverting this relation gives an exact explicit-unit definition of the mole in terms of the defining constant N_A

$$1 \text{ mol} = 6.022\,140\,76 \cdot 10^{23}/N_A \text{ (2)}$$

In order to comprehend from this formal SI definition what a mole actually means physically, we would need to have a firm concept of the meaning of the Avogadro constant or its reciprocal. Eq. (1) is no help in this respect, as this would involve pure circular reasoning.

For a sample of a substance X consisting of an aggregate of $N(X)$ atomic-scale chemically or otherwise equivalent entities, the SI Brochure describes the Avogadro constant as a dimensional proportionality constant, independent of the substance, relating the number of entities in the sample to the corresponding amount of the substance $n(X)$, as follows

$$N_A = N(X)/n(X) \text{ (3)}$$

The number of entities, $N(X)$, is easy to conceptualize even though its extremely large (integer) value would not be known precisely. But, since the mass of a sample of a substance, $m(X)$, is an aggregate of $N(X)$ atomic-scale entity masses

$$m(X) = N(X)m_a(X) = N(X)A_r(X) \text{ Da} \text{ (4)}$$

$N(X)$ can be *estimated* by dividing the total (easily measured) mass of the sample by the (known) entity mass of the substance

$$N(X) = m(X)/m_a(X) = m(X)/[A_r(X) \text{ Da}] \text{ (5)}$$

However, Eq. (3) for the meaning of N_A still seems to be incomprehensible unless we have a good understanding of the physical meaning of $n(X)$, i.e. the SI base quantity “amount of substance”.

But what is “amount of substance”? By their nature, *base* quantities cannot be defined (in terms of other quantities). However, the SI Brochure states that “Amount of substance, symbol n , is *defined* [emphasis added] to be proportional to the number of specified entities N in a sample, the proportionality constant being a universal constant” (i.e. “the same for all entities”), adding that this dimensional constant is the reciprocal of the Avogadro constant N_A , so that for any substance X

$$n(X) = N(X)/N_A \text{ (6)}$$

which is just an inversion of Eq. (3), again invoking circular logic. This relationship indicates that $n(X)$ here does not represent a “*base* quantity”, but rather the amount of a *particular sample of a specified* substance, i.e. a *quantity value*: the product of a (dimensionless) *number*, $N(X)$, and a substance-independent dimensional reference constant, $1/N_A$, which acts as a *unit*—according to quantity-calculus terminology (Taylor 2018).

Presumably, the base quantity is *amount*—a technical term—analogous to the base quantity *mass*, whereas $n(X)$ is analogous to the *quantity value* substance mass, $m(X)$, the mass of a particular sample

of the substance X given by Eq. (4). However, unlike the physical quantity mass—but very much like the physical quantity electric charge—amount is fundamentally discretized at the atomic scale.

The SI 2019 mole definition includes, *within* its formal statement—unique among base unit definitions—a sentence that attempts to *describe* the corresponding “base” quantity: “The amount of substance, symbol n , of a system is a measure of the number of specified elementary entities.” This does not help with understanding the meaning of the quantity. On the contrary, it is often mistakenly taken to mean that amount of substance is simply another name for the (dimensionless) number of entities, and that $n(X)$, when expressed in moles, is an alternative symbol for $N(X)$ —implying that “mole” is just another name for the (dimensionless) Avogadro number, in which case, the Avogadro constant would be a conversion factor, identically equal to unity (Brown, 2025). This sentence—as an integral part of the formal mole definition—adds yet another layer of confusion to the “mole concept” and related subjects.

Equation (6) is seen to be formally *compatible* with Eq. (2), i.e. (using N_{AvO} as the symbol for the Avogadro number), when $N(X) = N_{\text{AvO}}$ in Eq. (6), the right-hand side is $N_{\text{AvO}}/N_{\text{A}}$, which is one mole. But this does not help in forming a concept of amount of substance or its macroscopic unit from Eq. (2) because the Avogadro constant is still no less mysterious. This lack of clarity about N_{A} has been at the core of the widespread confusion permeating this subject for decades (Leonard 2016), now exacerbated by the circularity implied by the 2019 redefinition.

1.2 Dispelling the confusion: the elementary amount and the entity

In the following, I show how to break away from this circular reasoning by introducing the concept of the elementary amount n_{a} (Leonard 2025)—an amount consisting of a single atomic-scale entity of any substance (Morikawa and Newbold 2004)—analogous to the elementary charge, e (Job and Rüffler 2016). And I recommend adoption of the previously introduced (Leonard 2007) atomic-scale amount unit, the entity (symbol ent , dimension N), defined as exactly one elementary amount—paralleling the dalton (symbol Da , dimension M), currently defined as exactly one atomic mass constant, m_{u} . This means that substance amount, $n(X)$, is then easily conceptualized as an aggregate of a general number of atomic-scale entities, in which case the mole is seen to be an aggregate of a specified (Avogadro) number of entities (Leonard 2014). The Avogadro constant can then finally be understood—uniquely *defined* in terms of the elementary amount (n_{a}) and *expressed* in terms of the entity (ent), just as it can also be *expressed* in terms of the mole (mol), as in Eq. (1). Molar mass is shown to be the entity mass per entity, which (at the atomic scale) is self-evident. And the molar mass constant, M_{u} , is *exactly* equal to one dalton per entity (dimension M/N), which can be set equal to one gram per mole for all practical purposes—although this has theoretical implications, discussed in the appendix. Fundamental stoichiometric relationships selectively using atomic-scale and macroscopic units, seamlessly linking discrete and continuous regimes across the “Sorites threshold”, are summarized—as an alternative to confusing rote formulas based on opaque Factor-Label rules.

2. The elementary amount

2.1 A single atomic-scale entity

In order to escape from the loop of what appears to be circular logic that is at the root of so much confusion, consider a sample consisting of a single atomic-scale entity, the smallest possible *amount* of any substance (that retains that substance's chemical or other specified properties). From Eq. (6), we then have $n(X)|_{N(X)=1} = 1/N_A$. Since the right-hand side is independent of X , we do not have to indicate any specific kind of substance on the left. An amount consisting of a single atomic-scale entity of *any* substance (Morikawa and Newbold 2004) is then clearly an “elementary amount” (Job and Rüffler 2016, Leonard 2025). Like the elementary charge, e , the elementary amount is a physical constant of Nature; it has the dimension of amount, N . Following Morikawa and Newbold, with “ n ” representing amount and subscript “ a ” the atomic-scale, the most appropriate symbol for an amount of a single atomic-scale entity is n_a . Thus

$$n_a = 1/N_A \quad (7)$$

Significantly, this identifies a *reciprocal* Avogadro constant as the elementary amount.

2.2 Amount of substance understood

Now the relationship linking the amount of the substance $n(X)$ to the corresponding number of entities $N(X)$ in the sample given by Eq. (6) takes the form

$$n(X) = N(X)(1/N_A) = N(X) n_a \quad (8)$$

where the right-hand side is immediately recognized as an aggregate of $N(X)$ elementary amounts, directly paralleling the corresponding relationship for the total mass of the substance in the sample as an aggregate of $N(X)$ entity masses, Eq. (4)—one of the main differences being that $m_a(X)$ is substance dependent, whereas n_a is not.

2.3 Fundamental definition of the mole

The macroscopic unit of amount is now fundamentally *defined* (in terms of n_a) by setting $N(X)$ equal to the Avogadro number in Eq. (8)

$$1 \text{ mol} = N_{\text{Avo}} n_a \quad (9)$$

i.e. the mole is an aggregate of an Avogadro number of elementary amounts, which, given Eq. (7), clearly explains Eq. (2). It is important to stress that, since N_{Avo} is a (dimensionless) number, it is the elementary amount n_a that is the fundamental physical constant (dimension N) for the mole definition. But this is a reciprocal Avogadro constant, so that N_A itself (dimension $1/N$) can still be formally *designated* as the “defining constant” for the mole, as in Eq. (2)—just as the cesium frequency $\Delta\nu_{\text{Cs}}$ (dimension $1/T$), the

reciprocal of the cesium period (dimension T), is *designated* as the defining constant for the second (Leonard 2025).

It is instructive to summarize in one place the relationships for the number of entities in a sample, the corresponding amount of the substance, and the corresponding total mass of the substance, showing some clear parallels, as follows

$$N(X) = N(X)1 \quad (10)$$

$$n(X) = N(X) n_a \quad (11)$$

$$m(X) = N(X) m_a(X) \quad (12)$$

where 1 can be thought of as the “elementary number of entities” (dimension *number*, symbol 1); n_a is the (substance-independent) elementary amount (dimension *amount*, symbol N); and $m_a(X)$ is the (substance-dependent) entity mass (dimension *mass*, symbol M).

2.4 The Sorites paradox resolved

In principle, each of $N(X)$, $n(X)$, and $m(X)$ is a discrete-valued quantity value. Since $N(X)$ is an integer, the number of entities cannot be varied by less than 1. The amount of the substance cannot be varied by less than one elementary amount, n_a (just as macroscopic electric charge cannot be varied by less than one elementary charge, e). And the total substance mass in the sample cannot be varied by less than one atomic-scale entity mass, $m_a(X)$, on average (allowing for slight variations in isotopic composition). But at the macroscopic scale, all these quantity values are treated as continuous differentiable state variables.

This subject has been hotly debated by philosophers of science—specifically regarding $N(X)$ and especially $n(X)$, and whether the mole is a (dimensional) unit or a (dimensionless) number (Cooper and Humphrey 2010, Wheatley 2011a, Schmidt-Rohr 2020, Wolff 2020, Ghibaudi et al. 2024)—a classic example of the so-called Sorites paradox (Wheatley 2011b). The “paradox” is easily resolved, however: the state variables $N(X)$, $n(X)$ and $m(X)$ can all be *treated* as “continuous” whenever the number of entities in the sample is larger than that for which the addition or removal of one entity does not change the *measured* value of the variable of interest (to the precision used)—a basic axiom of continuum mechanics and thermodynamics. This measurement-instrument-dependent number is the “Sorites threshold”. This applies particularly to the total *mass* of the sample, since $N(X)$ is typically estimated *via* Eq. (5)—“counting by weighing”—and $n(X)$ is usually calculated from the (measured) mass value using the (known) molar mass of the substance: $n(X) = m(X)/M(X)$ —“amounting by weighing”.

2.5 Molar quantities at the atomic scale

In addition to equations (8) and (9) for clarifying the meaning of amount of substance and the mole, the elementary amount is useful for better understanding a number of other physical properties and

constants, traditionally involving products of the (poorly understood) Avogadro constant and atomic-scale quantities. For example, molar mass, defined as $M(X) = m(X)/n(X)$, is conventionally written as $N_A m_a(X)$. With N_A given by Eq. (1) and $m_a(X)$ expressed in grams or kilograms, this involves the product of an extremely large number of “reciprocal moles” and an extremely small mass value, which is not easily conceptualized. However, from equations (4) and (8), we see that

$$M(X) = m(X)/n(X) = [N(X)m_a(X)]/[N(X)n_a] = m_a(X)/n_a \quad (13)$$

immediately recognized as the entity mass per (amount of a single) entity.

Since $m_a(X) = A_r(X) m_u$ and $M(X) = A_r(X) M_u$, the molar mass constant M_u is seen from Eq. (13) to be the ratio of the atomic mass constant to the elementary amount, $M_u = m_u/n_a$ (dimension M/N)—rather than the non-intuitive conventional formula $N_A m_u$. Similarly, the molar gas constant R is equal to k/n_a , the Boltzmann constant per elementary amount, which is more easily understood as an atomic-scale quotient rather than $N_A k$ —again the product of a very large and a very small number when expressed in macroscopic units. And it is clear that k/n_a retains the same dimension as R . The Faraday constant F is e/n_a , intuitively recognized as the ratio of the elementary charge to the elementary amount—as opposed to the opaque product $N_A e$. These atomic-scale ratios should be compared with Schmidt-Rohr’s contention that $M_u = m_u$, $R = k$, and $F = e$, which is equivalent to setting n_a (and N_A) equal to 1. Finally, the molar Planck constant is related to the molar mass of carbon 12 by $h/n_a = K_C M(^{12}\text{C})$, where K_C is the coupling constant given by $K_C = c \alpha^2 A_r(e)/(24 R_{\infty}) = 3.325\,260\,5906(10) \cdot 10^{-8} \text{ m}^2/\text{s}$ (Leonard 2006), where the indicated uncertainty—dominated by that in α^2 —is the origin of the uncertainty now imbedded in the molar mass constant when expressed in macroscopic units. Currently, M_u is no longer exactly equal to 1 g/mol, although it can be set equal to this for almost all practical purposes. This is another source of confusion resulting from “compromises” made when constructing the 2019 redefinitions—specifically, by not redefining the dalton exactly in terms of the fixed- h kilogram (Leonard 2012).

3. Origin of the Avogadro number and evolution of the mole definition

3.1 The “gram-molecule”

Consider once again Eq. (5), written as

$$N(X) = m(X)/[A_r(X) \text{ amu}] \quad (14)$$

where “amu” is used here to represent the *chosen* atomic-scale mass unit used for cataloguing “atomic weights” at various periods of time—for example: $m_a(\text{H})$, $m_a(\text{O})/16$, or, more recently, $m_a(^{12}\text{C})/12$. Using the chemists’ traditionally preferred macroscopic mass unit, the gram, Eq. (14) can be rewritten as

$$N(X)/(g/\text{amu}) = m(X)/[A_r(X) \text{ g}] \quad (15)$$

where $A_r(X) \text{ g}$ is a *substance-dependent* reference mass—known, for any given substance, from a catalogue of “atomic weights,” $A_r(X) = m_a(X)/\text{amu}$. Long before the introduction of the mole, $A_r(X) \text{ g}$ was commonly called a “gram-atom” or “gram-molecule,” and described as the “atomic or molecular weight in grams.” It was sometimes called a “chemical mass unit” (Milton 2011)—although, being *substance dependent*, it is not a true *unit* (Thompson and Taylor 2008).

The significance of the gram-atom (gram-molecule, &c.) is that when the sample mass is equal to $A_r(X) \text{ g}$, the corresponding number of entities is seen from Eq. (15) to be equal to the (substance-independent) *constant* g/amu . So a sample of *any* substance with a mass of one gram-molecule was thereby known to contain the same number of particles as a sample of *any other* substance with a mass of one gram-molecule of that substance—the basis of Avogadro’s long neglected hypothesis involving equal volumes of gases (Brooke 1981). Perrin honored Avogadro by calling this (dimensionless) *invariable number* “Avogadro’s constant” (“constante d’Avogadro”) (Perrin 1909).

Prior to the redefinitions of SI base units in 2019, g/amu was *always* the definition of what was subsequently called the *Avogadro number*—involving the atomic-scale mass unit of choice (in any particular time period) used for cataloguing entity masses. For example: $g/m_a(\text{H}) \approx 5.98 \cdot 10^{23}$; $g/[m_a(\text{O})/16] \approx 6.022 \cdot 10^{23}$ —with a slight difference using the oxygen-16 isotope alone (Milton and Mills 2009). The carbon-12-based dalton gives $g/[m_a(^{12}\text{C})/12] \approx 6.0221 \cdot 10^{23}$.

3.2 The Avogadro number is the quotient of two mass units

The *Avogadro number* is not a “constant of Nature.” Rather, its numerical value derives from the *choice* of two designated mass units, the gram and the dalton. If entity masses used in stoichiometry were catalogued in yoctograms instead of daltons, so that $m_a(X) = A_r^*(X) \text{ yg}$, the “Avogadro number”—i.e. the number of entities in a sample corresponding to a mass of $A_r^*(X) \text{ g}$ —would be (exactly) $1 \cdot 10^{24}$. The “mole” would be an aggregate of (exactly) $1 \cdot 10^{24}$ elementary amounts, and the “Avogadro constant” would be (exactly) one per “yoctomole” ($= 10^{24}$ per “mole”). The *Avogadro number* is also totally *independent* of the (confusingly named) *Avogadro constant*. The latter, fundamentally *defined*—by inverting Eq. (7)—as one per elementary amount (Leonard 2025), can be *expressed* as an “Avogadro number per mole”, and the Avogadro number can be *described* as the “number of entities in one mole”—but this is because the mole is *defined* in terms of the Avogadro number (and the elementary amount) as in Eq. (9), not the other way around.

3.3 The 2019 redefinition of the mole

In terms of the elementary amount, the pre-2019 definition of the mole (although not written this way) was always of the form

$$1 \text{ mol} = (g/\text{amu}) n_a \quad (16)$$

Just prior to the 2019 redefinitions—of both the mole *and* the kilogram—one mole was therefore given by $(\text{g/Da}) n_a = \{(0.001 \text{ kg})/[m_a(^{12}\text{C})/12]\}n_a$, or $0.012 m(\text{IPK})/[m_a(^{12}\text{C})/n_a]$. From Eq. (13), this is $0.012 m(\text{IPK})/M(^{12}\text{C})$, involving two defining constants: the kilogram prototype and the molar mass of carbon 12 (Taylor 2018).

The CODATA 2018 value of the dalton in terms of the fixed-Planck-constant kilogram was $\text{Da} = 1.660\,539\,066\,60(50) \cdot 10^{-27} \text{ kg}$ (Tiesinga et al. 2021). So that gram-to-dalton ratio was $(\text{g/Da})_{2018} = 6.022\,140\,7620(18) \cdot 10^{23}$. This value, rounded to nine significant figures, thus guaranteeing continuity to the precision shown, was then *chosen* as the fixed exact value assigned to the Avogadro *number*, N_{AvO} , used in the 2019 redefinition of the mole.

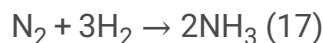
The measured value and uncertainty of $\text{g/Da} = (0.012 \text{ kg})/m_a(^{12}\text{C})$ will both change slightly with each new CODATA adjustment of the carbon-12 atomic mass value in terms of the fixed- h kilogram. For example, the subsequent CODATA 2022 value for the dalton was listed as $\text{Da} = 1.660\,539\,068\,92(52) \cdot 10^{-27} \text{ kg}$ (Mohr et al. 2025), resulting in a value of $(\text{g/Da})_{2022}$ that differs from the fixed N_{AvO} value by a relative term of order 10^{-10} —which, given the uncertainties inherent in stoichiometric mass measurements, is negligible for all practical purposes.

The 2019 redefinition of the mole is still in the form of Eq. (9) but N_{AvO} is now fixed at an exact value. However, the retained carbon-12-based dalton (meaning that g/Da is no longer *exactly* equal to N_{AvO}) has introduced yet another subtle layer of confusion, transmitting the (extremely small) uncertainty in the earlier carbon-12-based Avogadro number to the molar mass constant M_u (equal to m_u/n_a exactly, but not quite exactly equal to 1 g/mol).

4. The appropriate atomic-scale amount unit

4.1 Atomic-scale amounts in yoctomoles

Consider the following chemical reaction for the synthesis of ammonia, where at the atomic scale, one molecule of diatomic nitrogen reacts with three molecules of diatomic hydrogen to produce two molecules of ammonia



The atomic-scale number of nitrogen molecules involved in the nominal reaction (with minimized integer coefficients) is $N_1(\text{N}_2) = 1$. Similarly, $N_1(\text{H}_2) = 3$ and $N_1(\text{NH}_3) = 2$. Since the change in the atomic-scale amount of each component, $\Delta n_1(X)$, is the (signed) change in the respective number of entities divided by N_A , we see that for nitrogen: $\Delta n_1(\text{N}_2) = -1/N_A =$

$-1/(6.022\,140\,76 \cdot 10^{23} \text{ mol}^{-1}) \approx -1.66 \cdot 10^{-24} \text{ mol}$, or -1.66 yoctomoles. For hydrogen: $\Delta n_1(\text{H}_2) \approx -4.98 \text{ ymol}$. And for ammonia: $\Delta n_1(\text{Al}_2\text{Br}_6) \approx +3.32 \text{ ymol}$. The same results could have been obtained by dividing each atomic-scale component mass expressed in daltons by its respective molar mass given by

$$M(X) = m(X)/n(X) = A_r(X)N_A \text{ Da} \approx 0.6022 A_r(X) \text{ Da/ymol} \quad (18)$$

Although the yoctomole *could* be used as the atomic-scale unit for amount of substance, as the above example shows, the introduction of the poorly understood Avogadro constant (as approximately 0.6022 per yoctomole) creates an unnecessary degree of complexity. It would be much less confusing to introduce an amount unit more appropriately representative of the amounts of individual entities themselves—just as the dalton (rather than approximately 1.66 yoctograms) is an appropriate atomic-scale mass unit representative of the mass of a single proton or neutron.

4.2 The atomic-scale amount unit: entity, symbol ent

In the above example, rather than using the term “molecule,” we could use the generic term “entity” and say that an amount of one entity of diatomic nitrogen reacts with an amount of three entities of diatomic hydrogen to produce an amount of two entities of ammonia. And this terminology would be appropriate and easily comprehended, no matter what kinds of atomic-scale entities were involved. This of course means that “entity” is the appropriate name for such an atomic-scale amount *unit*—and “ent” is then clearly a suitable symbol (Leonard 2007, 2010b, 2011, 2014). Since the elementary amount, n_a , is a physical *quantity value* representing the amount of a single entity of any kind, the *unit* entity, ent, must be defined as

$$1 \text{ ent} = n_a \text{ (dimension N)} \quad (19)$$

This parallels the situation with the *unit* dalton, Da, and the atomic-scale reference mass *quantity value* $m_a(^{12}\text{C})/12$, known as the atomic mass constant, m_u

$$1 \text{ Da} = m_u \text{ (dimension M)} \quad (20)$$

It should be emphasized that the name entity and symbol ent, from the original definition (Leonard 2007) refer to a *bona fide* (dimensional) physical unit with the dimension of amount of substance N, not a (dimensionless) pseudo-unit—i.e. not a “special name for the number one” (Leonard 2015, Leonard 2025) as later proposed (Mohr and Phillips 2015) and again more recently (Kacker 2025).

4.3 The fundamental relationship between $n(X)$ and $N(X)$ —at any scale

From Eq. (8), we can now *express* the amount of substance in a sample in terms of the (atomic-scale *unit*) entity as

$$n(X) = N(X) \text{ ent} \quad (21)$$

—an aggregate of $N(X)$ entities—demonstrating that “amount of (a specified) substance,” $n(X)$, is indeed a quantity value, the product of a number and a unit (Taylor 2018), rather than a base quantity. Note that, just as $m(X)/g$ is “the number of grams” in a particular sample, $n(X)/\text{ent}$ is correctly called “the number of entities” in the sample—i.e. $N(X)$ —further validating the selection of the term “entity” for the name of this unit.

The macroscopic unit, now easily conceptualized as an aggregate of an Avogadro number of entities, can be *expressed* directly in terms of the atomic-scale unit

$$1 \text{ mol} = N \text{ ent} \quad (22)$$

where $N_{\text{Avo}} (= \text{mol}/\text{ent} = 6.022\,140\,76 \cdot 10^{23})$ links the macroscopic and atomic-scale amount units from discrete to continuous realms across the Sorites threshold. Then substance amount can be expressed in terms of the mole as

$$n(X) = [N(X)/N_{\text{Avo}}] (N_{\text{Avo}} \text{ ent}) = [N(X)/N_{\text{Avo}}] \text{ mol} \quad (23)$$

—again the product of a number and (in this case) a macroscopic unit. Note that “the number of moles” in a sample is $n(X)/\text{mol}$ (dimension $N/N = 1$). The ubiquitous (incorrect) use of this phrase as a substitute for “the amount” of the given substance should be strongly deprecated.

4.4 The Avogadro constant (finally) understood

Now the Avogadro constant, fundamentally *defined* (uniquely) as one per elementary amount

$$N_{\text{A}} = 1/n_{\text{a}} \quad (24)$$

independently of any chosen amount unit, can be *expressed* in terms of the atomic-scale amount unit as

$$N_{\text{A}} = 1/\text{ent} \quad (25)$$

in addition to being *expressed* in terms of the macroscopic amount unit, $N_{\text{A}} = N_{\text{Avo}}/\text{mol}$, as in Eq. (1). The *definition* of N_{A} as “one per elementary amount” and its *expression* as “one per entity” at last gives us the correct concept of what the Avogadro constant really means—but it is not usually needed because the more easily conceptualized elementary amount (n_{a}) or the more appropriately sized atomic-scale amount unit entity (ent)—each with the dimension N —can always be used instead of the reciprocal Avogadro constant, with the less intuitive dimension of $1/N$. (Job and Rüffler use τ as the “Elementare Stoffmenge” almost exclusively instead of $1/N_{\text{A}}$). This is seen here, for example, in equations (8), (9), (13), (21) and (22).

5 Stoichiometry

5.1 Molar mass in atomic-scale and macroscopic units

From Eq. (13) but now in terms of the unit entity, molar mass is given by

$$M(X) = [N(X)m_a(X)]/[N(X) \text{ ent}] = m_a(X)/\text{ent} \quad (26)$$

which is easily understood as one entity mass per (unit) entity, dimension M/N. And, since $m_a(X) = A_r(X)$ Da, $M(X)$ can be written entirely in terms of atomic-scale units (*exactly*) as

$$M(X) = A_r(X) \text{ Da/ent} \quad (27)$$

where dalton per entity is the appropriate atomic-scale unit for this *intensive property* of a substance (dimension M/N). This means that the molar mass constant, $M_u = M(X)/A_r(X) = m_u/n_a$ is (exactly) one dalton per entity. Assuming that N_{AvO} can be set equal to g/Da (for all practical purposes), one dalton per entity can be written as $[(\text{g/Da}) \text{ Da}]/(N_{\text{AvO}} \text{ ent}) = \text{g/mol}$, so that (to high precision)

$$M_u \equiv 1 \text{ Da/ent} = 1 \text{ g/mol} \equiv 1 \text{ kg/kmol} \quad (28)$$

The use of the entity (ent) here is important in maintaining dimensional consistency: $\dim[\text{Da/ent}] = \dim[\text{g/mol}] = \text{M/N}$. Whereas, equating Da (dimension M) to g/mol (dimension M/N)—as seen in some textbooks, online tutorials and journal articles when introducing the concept of molar mass (Schmidt-Rohr 2020)—is a confusing violation of dimensional homogeneity rules.

5.2 Number, amount and mass relationships

Equations (10)–(12) can now be combined in terms of the units one, entity, and dalton, for the number of entities, the substance amount, and the substance mass, appropriate at the atomic-scale

$$N(X)/1 = n(X)/\text{ent} = [m(X)/A_r(X)]/\text{Da} \quad (29)$$

In terms of the macroscopic units, mole and gram—again assuming that $N_{\text{AvO}} = \text{g/Da}$ (for all practical purposes)

$$N(X)/N_{\text{AvO}} = n(X)/\text{mol} = [m(X)/A_r(X)]/\text{g} \quad (30)$$

and this formula can be extended, when appropriate, to the corresponding volume of an ideal gas at a given pressure and temperature.

5.3 Atomic-scale amounts $\Rightarrow$ macroscopic stoichiometric ratios

Returning to the example of the ammonia synthesis reaction, now using the entity as the appropriate amount unit, we see that the *changes* in the respective atomic-scale amounts indicated by one run of the conversion relation at the atomic scale are clearly given in terms of this unit

$$\Delta n_1(\text{N}_2) = -1 \text{ ent} \quad (31)$$

$$\Delta n_1(\text{H}_2) = -3 \text{ ent (32)}$$

$$\Delta n_1(\text{NH}_3) = +2 \text{ ent (33)}$$

—which is much more intuitively obvious than working with multiples of 1.66 yoctomoles. Here, the important concept of the *atomic-scale* extent of reaction is given by

$$\xi_1 = 1 \text{ ent (34)}$$

So we see that

$$\xi_1 = -\Delta n_1(\text{N}_2)/1 = -\Delta n_1(\text{H}_2)/3 = +\Delta n_1(\text{NH}_3)/2 \text{ (35)}$$

If N_{tot} is the total number of atomic-scale reactions involved in the macroscopic reaction, then the change in each macroscopic amount is of the form $\Delta n(\text{X}) = N_{\text{tot}} \Delta n_1(\text{X})$. Thus

$$\Delta n(\text{N}_2) = -N_{\text{tot}} \text{ ent} = -\xi \text{ (36)}$$

$$\Delta n(\text{H}_2) = -3N_{\text{tot}} \text{ ent} = -3\xi \text{ (37)}$$

$$\Delta n(\text{NH}_3) = +2N_{\text{tot}} \text{ ent} = +2\xi \text{ (38)}$$

where ξ is the (macroscopic) extent of reaction. By definition, this is

$$\xi = N_{\text{tot}} \xi_1 = N_{\text{tot}} \text{ ent} = (N_{\text{tot}}/N_{\text{Avo}}) \text{ mol (39)}$$

where the macroscopic unit of extent of reaction, the mole, is seen to appear quite naturally.

Then we have the fundamental stoichiometric relationships

$$\xi = -\Delta n(\text{N}_2)/1 = -\Delta n(\text{H}_2)/3 = +\Delta n(\text{NH}_3)/2 \text{ (40)}$$

equating the changes in macroscopic amounts of each component in this reaction scaled by their respective (signed) stoichiometric numbers.

The introduction of the atomic-scale amount unit entity makes perfectly clear *why* the changes in amounts of *any* two components (reactants or products) X and Y are in the same ratio as their respective stoichiometric numbers ν_X and ν_Y . Generalizing from the above example, we can write $\Delta n(\text{X}) = \nu_X \xi$ and $\Delta n(\text{Y}) = \nu_Y \xi$. Then, since $\xi = \Delta n(\text{X})/\nu_X = \Delta n(\text{Y})/\nu_Y$, the macroscopic amount quotient of any two components is exactly equal to the respective stoichiometric number quotient

$$\Delta n(\text{X})/\Delta n(\text{Y}) = \nu_X/\nu_Y \text{ (41)}$$

Using either Eq. (29) or (30), this can be extended to the respective numbers of entities and sample masses of the two components

$$\Delta N(X)/\Delta N(Y) = \Delta n(X)/\Delta n(Y) = [\Delta m(X)/A_r(X)]/[\Delta m(Y)/A_r(Y)] = v_X/v_Y \quad (42)$$

For ideal gases, the ratio of changes in volume $\Delta V(X)/\Delta V(Y)$ —at a given temperature and pressure—is also equal to v_X/v_Y . If only masses are of primary interest, these are directly related by

$$\Delta m(X)/\Delta m(Y) = [v_X A_r(X)]/[v_Y A_r(Y)] \quad (43)$$

These stoichiometric-ratio relationships are based on sound physical principles. Their derivation here, at first involving the extent of reaction at the atomic scale—stemming from using the intuitively clear amount unit entity when describing amounts of each component involved in the atomic-scale reaction—then seamlessly scaled up to macroscopic amounts in terms of the mole, is far easier for students to understand than opaque rote calculation rules involving the ubiquitous Factor-Label method and so-called “conversion factors.” Legitimate conversion factors are identically equal to 1, so these rote rules continue to cause further confusion (Dunphy and Weisse 2025) by appearing to imply that a mole is either a number (the Avogadro number) or a mass, $A_r(X)$ g, and that an amount of “ v_X moles of X” is somehow *chemically equivalent* to or can be *converted* to an amount of “ v_Y moles of Y” involving so-called “mole-ratio conversion factors.”

6 Summary and conclusions

Given the atomic structure of matter and the fact that mass is an additive physical quantity, it is easy for STEM students to conceptualized the quantity value representing the macroscopic mass of a sample of a substance as an aggregate of a (very large) number of (very small) atomic-scale entity masses: $m(X) = N(X) m_a(X)$ —where $m_a(X)$ is catalogued in terms of an appropriate atomic-scale mass unit, the dalton. Although entity masses are discrete, the number of entities in a macroscopic sample is so large that both $N(X)$ and $m(X)$ can be treated as continuous differentiable state variables.

However, when it comes to the corresponding amount of the substance in the sample, $n(X)$, this is much more difficult to conceptualize, particularly because it *is defined* by the SI as being proportional to (or, according to the formal definition of the mole, *a measure of*) $N(X)$, where the (substance-independent) dimensional proportionality constant is the reciprocal of the so-called “Avogadro constant,” i.e. $n(X) = N(X)/N_A$. This constant, in turn, is *defined* by the SI as $N_A = N(X)/n(X)$ —which is purely circular.

The resulting widespread confusion about the “mole concept” and related subjects could be entirely eliminated simply by paralleling the situation with substance mass—i.e. by recognizing the existence of an amount of a single entity as the elementary amount, analogous to the mass of a single entity (and, more appropriately, to the elementary charge), and adopting a currently absent atomic-scale amount unit representative of (in fact, equal to) that elementary amount, analogous to the dalton as the atomic-scale mass unit.

The introduction of the elementary amount, n_a , the smallest possible amount of any substance, and the corresponding atomic-scale amount unit, the entity, $1 \text{ ent} = n_a$, means that the amount (of a substance X) in a sample is a quantity value that can be *related* explicitly to $N(X)$ as $n(X) = N(X) n_a$ and *expressed* as a well-defined quantity value: $n(X) = N(X) \text{ ent}$ —the product of a number and a unit. Then $n(X)$ is easily conceptualized as an aggregate of $N(X)$ individual entities, paralleling substance mass as an aggregate of $N(X)$ entity masses. Again, because $N(X)$ is so large in a macroscopic sample, $n(X)$ is treated as a continuous state variable.

The macroscopic amount unit is *defined* as: $1 \text{ mol} = N_{\text{Avo}} n_a = N_{\text{Avo}} \text{ ent}$. And, for all practical purposes, the corresponding sample mass is $A_r(X) \text{ g}$ —a “gram molecule”—thereby retaining the original concept of the mole. Molar mass can be written, at the atomic scale as $M(X) = m_a(X)/n_a = m_a(X)/\text{ent} = A_r(X) \text{ Da}/\text{ent} = A_r(X)M_u$. The molar mass constant is *exactly* equal to one dalton per entity and, in practice, this can be set equal to one gram per mole or one kilogram per kilomole, consistently retaining the dimension M/N across the entire discrete-to-continuous spectrum.

Just as the dalton is the appropriate mass unit when relatively small masses are involved, the entity is a much more appropriate amount unit than the mole when relatively small amounts are involved, especially in very dilute amount concentrations, thereby avoiding the use of pseudo-units or awkward submultiples of the mole. In statistical mechanics, polymer chemistry, biochemistry, nanotechnology and quantum chemistry—i.e. within the discrete-entity realm—the use of the atomic-scale unit ent retains the dimension N, rather than *suddenly switching* to a dimensionless (integer) count of individual entities below the Sorites threshold. Many other aspects of the “mole concept” and related subjects are thereby greatly clarified. Stoichiometric relationships can be put on a sound physical basis and introduced earlier in the physical-chemistry curriculum, instead of relying on poorly understood rote calculation formulas. It should be remarked that, apart from its appearance as the designated defining constant in the formal SI definition of the mole, the confusingly named “Avogadro constant”—defined as $N_A = 1/n_a$ and expressed as $N_A = 1/\text{ent} = N_{\text{Avo}}/\text{mol}$ —could be said to be largely irrelevant.

Finally, reviewing equations (10), (11), and (12), it is important to remember that *all* of $N(X)$, $n(X)$, and $m(X)$, just like electric charge, are fundamentally discretely valued physical quantities, that can be *treated* as continuous, differentiable state variables in macroscopic samples (i.e. above the Sorites threshold), depending entirely on the particular measurement precision in use—especially for $m(X)$, from which $N(X)$ and $n(X)$ are usually calculated: “counting” and “amounting” by weighing. Hopefully this will put to rest (ongoing) debates about the dimension of the mole and the legitimacy of “the-quantity-of-which-it-is-the-unit” by emphasizing that, in a Shakespearean-style rhyming couplet: Without an amount, there is nothing to count!

Declarations

Author Contribution

B.L. wrote the entire manuscript.

References

1. Atkins, P., de Paula, J., Keeler, J.: *Atkins' Physical Chemistry* (12th ed.). Oxford University Press: (2023)
2. BIPM. The International System of Units (SI) (9th ed.). Sèvres: (updated (2019)
3. v3.02–August 2025)
4. Brooke, J.H.: Avogadro's hypothesis and its fate: A case study in the failure of case-studies
5. Hist: Sci. **19**, 235–273 (1981)
6. Brown, R.J.C.: Comment on The Avogadro constant is not the defining constant of the mole
7. Metrologia: 62, No. 058004 (2025)
8. Cooper, G., Humphrey, S.M.: The ontological distinction between units and entities. *Synthese*. **187**, 393–401 (2010)
9. Dunphy, S., Weisse, Z.: Replacement of Dimensional Analysis with Proportional Reasoning in
10. Introductory Chemistry and: its Effects on Students' Chemistry Conceptual understanding. *J. Chem. Educ.* **102**, 1788–1802 (2025)
11. Fang, S.-C., Hart, C., Clarke, D.: Unpacking the Meaning of the Mole Concept for Secondary
12. School Teachers and Students: *J. Chem. Educ.* **91**, 351–356 (2014)
13. Furio, C., Azcona, R., Guisasola, J.: The Learning and Teaching of the Concepts Amount of
14. Substance and: A Review of the Literature. *Chem. Educ. Res. Pract.* **3**, 277–292 (2002)
15. Ghibaudi, E., Ghirardi, M., Regis, A.: Are there distinct views of chemistry behind the old and
16. the new definition of mole?: *Found. Chem.* **26**, 385–398 (2024)
17. Job, G., Rüffler, R.: *Physical Chemistry from a Different Angle: Introducing Chemical*
18. Equilibrium: *Kinetics and Electrochemistry by Numerous Experiments*. (1st ed.). Springer, Cham. (2016)
19. Kacker, R.N.: Reply to Comment on The Avogadro constant is not the defining constant of the
20. mole: *Metrologia* 62 No 058001 (2025)
21. Kacker, R.N., Irikura, K.K.: The Avogadro constant is not the defining constant of the mole
22. *Metrologia*, 62: No. 013003 (2025a)
23. Kacker, R.N., Irikura, K.K.: The SI unit mole and Avogadro constant. *Measurement: Sens.* **38**, e1–e4 (2025b)
24. Leonard, B.P.: Note on invariant redefinitions of SI base units for both mass and amount of
25. substance. *Metrologia* 43, L3–L5: (2006)
26. Leonard, B.P.: The atomic-scale unit, entity: key to a direct and easily understood definition of
27. the SI base: unit for amount of substance. *Metrologia*. **44**, 402–406 (2007)

29. Leonard, B.P.: Comments on recent proposals for redefining the mole and kilogram. *Metrologia*. **47**, L5–L8 (2010a)
30. Leonard, B.P.: Why the invariant atomic-scale unit, entity, is essential for understanding
31. stoichiometry without: *Accred Qual. Assur.* **16**, 133–141 (2010b)
32. Leonard, B.P.: Alternative interpretations of the mole and the ideal gas equation. *Accred. Qual*
33. *Assur*: **16**, 577–581 (2011)
34. Leonard, B.P.: Why the dalton should be redefined exactly in terms of the kilogram. *Metrologia*. **49**, 487–491 (2012)
35. Leonard, B.P.: The mole is an Avogadro number of entities, the macroscopic unit for chemical
36. amount. *Accred Qual. Assur.* **19**, 213–220 (2014)
37. Leonard, B.P.: Comment on Dimensionless units in the SI. *Metrologia*. **52**, 613–616 (2015)
38. Leonard, B.P.: Why is amount of substance so poorly understood? The mysterious Avogadro
39. constant is the culprit: *Accred Qual. Assur.* **21**, 231–236 (2016)
40. Leonard, B.P.: Second comment on The Avogadro constant is not the defining constant of the
41. mole: *Metrologia* 62 No 058003 (2025)
42. Mills, I.M., Mohr, P.J., Quinn, T.J., Taylor, B.N.: Williams, E. R.: Redefinition of the
43. kilogram, ampere, kelvin and mole: a proposed approach to implementing CIPM recommendation 1
- (CI–2005). *Metrologia* 43, 227–246 (2006)
44. Milton, M.J.T.: A new definition for the mole based on the Avogadro constant: a journey from
45. physics to chemistry: *Philos. Trans. Roy Soc. A.* **369**, 3993–4003 (2011)
46. Milton, M.J.T., Mills, I.M.: Amount of substance and the mole. *Chimia*. **63**, 613–621 (2009)
47. Mohr, P.J., Phillips, W.D.: Dimensionless units in the SI. *Metrologia*. **52**, 40–47 (2015)
48. Mohr, P.J., Newell, D.B., Taylor, B.N.: Tiesinga, E.: CODATA recommended values of the
49. fundamental physical constants: *Phys. Chem. Ref. Data* 54, No. 033105 (2025). (2022) J
50. Morikawa, T., Newbold, B.T.: Amount of substance and a single elementary entity
51. *Khimiya/Chemistry: (Bulg J. Chem. Educ).* **13**, 431–435 (2004)
52. Moss, K., Pabari, A.: The Mole Misunderstood. *New Directions in the Teaching of Natural*
53. *Sciences*: **6**, 77–86 (2016)
54. Pekdağ, B., Azizoğlu, N.: Semantic Mistakes and Didactic Difficulties in Teaching the Amount
55. of Substance.: *Chem. Educ. Res. Pract.* **14**, 117–129 (2013)
56. Perrin, J.B.: *Brownian Movement and Molecular Reality*; Soddy, F., Transl.; Taylor and Francis
57. London: originally published as Mouvement brownien et réalité moléculaire. *Ann. Chim. Phys.* **18**, 5–114 (1909). (1910)
58. Rees, S.W., Bruce, M.: Inconsistent Language Use in Online Resources Explaining the Mole
59. Has Implications for Students' Understanding: *J. Chem. Educ.* **99**, 2446–2450 (2022)

60. Schmidt-Rohr, K.: Analysis of Two Definitions of the Mole That Are in Simultaneous Use, and
61. Their Surprising Consequences: J. Chem. Educ. **97**, 597–602 (2020)
62. Taylor, B.N.: Quantity calculus, fundamental constants, and SI units. J. Res. Natl. Inst. Stan
63. Technol. 123, No. 123008: (2018)
64. Thompson, A., Taylor, B.N.: *Guide for the use of the International System of Units (SI)*; NIST
65. Special Publication 811; National Institute of Standards and Technology: Gaithersburg, MD: (2008)
66. Tiesinga, E., Mohr, P.J., Newell, D.B.: Taylor, B. N.: CODATA recommended values of the
67. fundamental physical constants: Rev. Mod. Phys. 99, No. 025010 (2021). (2018)
68. Wheatley, N.: On the dimensionality of the Avogadro constant and the definition of the mole
69. Metrologia: 48, 71–82 (2011a)
70. Wheatley, N.: A Sorites paradox in the conventional definition of amount of substance
71. Metrologia, 48: L17–L21 (2011b)
72. Wolff, J.E.: Heaps of moles? Mediating macroscopic and microscopic measurement of chemical
73. substances. Stud. Hist. Phil Sci. **80**, 19–27 (2020)

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