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Commentary

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The Mole and Amount of Substance in Chemistry and Education: Beyond Official Definitions

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ABSTRACT: The definition of the mole in the current SI and the draft definition for the "new SI" are reviewed. Current textbook treatments of the mole are compared to these official definitions. For historical perspective, the treatment of the mole and *amount of substance* in textbooks before and after those quantities were introduced into the SI in 1971 is reviewed. Textbook definitions have not always matched the official definitions, but they reflect the common usage of chemists. Textbook definitions will likely resemble the official definition more closely if the new SI is adopted, because the draft definition is closer than the current official definition to what is found in many textbooks. The SI base quantity *amount of substance*, however, will likely continue to pose problems for chemistry educators and to be widely ignored by practitioners of chemistry if it is retained. Official definitions and expert usage of some terms related to the mole (particularly *amount of substance*) do not always coincide.

KEYWORDS: *First-Year Undergraduate/General, High School/Introductory Chemistry, History/Philosophy, Nomenclature/Units/Symbols, Stoichiometry*

■ INTRODUCTION

The General Conference on Weights and Measures (CGPM) has proposed to revise the International System of Units (SI) so that all of its base units will be defined by "explicit-constant" formulations.[1] Draft definitions for the "new SI"[2] of two units in particular have received scrutiny from chemists, namely, the mole and the kilogram. For example, the ACS Committee on Nomenclature, Terminology, and Symbols has been monitoring proposals on these units for several years, sponsoring symposia on the subject at national meetings and publishing comments in *Chemical and Engineering News*.[3,4]

This article focuses on the current definition of the mole,[5] as well as the definition contained in the 2013 draft brochure of the new SI,[2] with an eye toward teaching the mole in introductory chemistry classes. Some current textbooks are examined for how they teach about the mole in order to compare the official definition to current educational practice. In order to put the likely effects of the proposed change into historical perspective, a comparison is made to effects from an earlier major change in SI for chemists, namely, the inclusion of the mole as an SI base unit in 1971.

■ THE MOLE IN CURRENT TEXTBOOKS

The mole is key content in every introductory chemistry textbook, and teaching the mole is a perennial subject in chemistry education. The current official definition of the mole reads[5]

> *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; its symbol is "mol".*

Here is the definition given in the 2013 draft of the new SI:[2]

> *The mole, symbol mol, is the SI unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles; its magnitude is set by fixing the numerical value of the Avogadro constant to be exactly 6.022 141 29 × 10^{23} when it is expressed in the SI unit mol^{-1}.*

Now let us have a look at how the mole is defined in the glossaries of some recent textbooks (presumably under the influence of the current SI):

- Gilbert et al. ("2015"): Their definition looks more like the new SI than the old, although the terminology is not exactly the same as either: "an amount of material (atoms, ions, or molecules) that contains Avogadro's number[6] (N_A = 6.022 × 10^{23}) of particles."[7]
- Tro (2011) is quite similar: "A unit defined as the amount of material containing 6.0221421 × 10^{23} (Avogadro's number) particles."[8]
- Silberberg (2013) uses the current SI definition: "The SI base unit for amount of a substance. The amount that contains a number of objects equal to the number of atoms in exactly 12 g of carbon-12 (which is 6.022 × 10^{23})."[9]

The treatment within the body of a textbook includes examples, and relates the mole to mass as well as number of entities. Here is how Nivaldo Tro introduces the topic in the body of his textbook, in a section titled "The Mole: A Chemist's 'Dozen'":[8]

> *A mole is the amount[10] of material containing 6.02214 × 10^{23} particles.*
> *1 mol = 6.02214 × 10^{23} particles*
> *This number is also called **Avogadro's number**...*
> *... Notice that the definition of the mole is an amount of substance. We will often refer to the number of moles of substance as the amount of the substance.*

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This passage refers to *amount of substance*, which officially is the name of the quantity of which mole is the base unit. It does not, however, treat amount of substance as a technical term, but rather as an explanatory phrase: "Notice that" it is "an" amount. The section goes on to emphasize that the mole can specify Avogadro's number of anything.

The next paragraph says[8]

The second, and more fundamental, thing to understand about the mole is how it gets its specific value.
The value of the mole is equal to the number of atoms in exactly 12 grams of pure carbon-12 (12 g C = 1 mol C atoms = 6.022×10^{23} C atoms).

Here some of the language of the current SI definition is incorporated. But the wording of the sentence that refers to carbon-12 speaks tellingly about "the value of the mole", practically equating the unit with Avogadro's number.

Comparing the draft definition of the mole to current textbook treatments suggests two implications:

1. Textbook definitions of the mole as a definite number of elementary entities—already common—would appear closer to the new, proposed official SI definition, even if textbooks retain explicit-unit formulations and continue to refer to Avogadro's number.
2. The draft retains a stumbling block to understanding, the term *amount of substance.*

■ A LOOK BACK: THE MOLE ENTERS SI

The expectation that textbooks of the future will not change their definitions of the mole very much in response to the change in the SI definition is based partly on the fact that the draft SI is in some respects closer than the current definition to what many textbooks have already. But it is also based on the fact that textbooks did not greatly change how they introduced the mole over the years.

Consider textbook definitions from before the inclusion of the mole into the SI. The term and unit mole had been in use in chemistry since roughly the start of the 20th century;[11] however, it was incorporated into the SI as a base unit, along with the base quantity *amount of substance* only in 1971. The following statements are all from textbooks published in the 1960s:

- Selwood (1964): "The word 'mole' is a collective noun like flock (of birds) or galaxy (of stars). But mole has the added meaning of a very definite number of particles, namely, Avogadro's number."[12]
- Andrews & Kokes (1965): "... *the weight of a single molecule in atomic mass units is the same, numerically, as the weight of a mole in grams. The mole is a convenient package, like a dozen or a gross; but numerically it is much larger.*" A footnote contains something closer to what would be adopted as the SI definition: "A mole is a number equal to the number of atoms in exactly twelve grams of C^{12} (6.02252×10^{23})..."[13,14]
- Kask (1969): "The number, 6.02×10^{23}, is known as a *mole*. This number is also known as Avogadro's number..."[15]

Compare the above definitions to the following, from textbooks of the late 1970s and early 1980s, several years *after* the inclusion of the mole into the SI.

- Masterton and Slowinski (1977): "In discussing mass relations in chemical reactions, we make frequent use of a quantity known as the **mole**. Depending upon the context in which the word 'mole' is used, it may refer to a specific number of particles or to a specific mass in grams. That is, it may represent: (1) **Avogadro's number of items**... (2) **One gram formula weight of a substance**..."[16]
- Becker and Wentworth (1980): "So that we can ultimately give the relative masses of substances in units of grams, we define a *mole* (mol) as *Avogadro's number* (N) of particles. ... Thus a mole can be further defined as ... the quantity of a substance the mass of which is the atomic or molecular weight (including formula weight) in grams."[17]
- Mortimer (1983) uses language very similar to the SI definition: "The amount of a substance that contains Avogadro's number [previously defined] of elementary units is called a mole (abbreviated mol), which is an SI base unit. The mole is defined as the amount of substance that contains as many elementary entities as there are atoms in exactly 12 g of carbon-12."[18]

Mortimer happens to be the last example selected from this time period, but I do not want to imply that eventually textbook authors followed his example and adopted the official SI definition; examining recent textbooks (as done above) shows that this is not the case. Indeed, this glimpse at how the mole has been described in textbooks over the past 50 years or so suggests that textbook authors have emphasized throughout that a mole contains a definite number of entities. If the draft definition of the mole in the "new SI"[2] is adopted, textbook definitions will likely resemble it more closely not because they will move toward the official definition but because the official definition will have moved closer to the textbooks (albeit not for pedagogical purposes).

■ OF OFFICIAL DEFINITIONS AND TEXTBOOKS

It may be that textbooks will not adapt to or reflect changes in official definitions of the SI. That would not necessarily be an unfortunate development. After all, official definitions

- Are formal, not pedagogical, by design
- Do not necessarily represent a consensus of relevant practitioners
- Are not Platonic ideas coextensive with the things they define

Let us look more closely at these assertions in the light of current practices and a few examples from the pedagogical literature. Having concentrated above on the mole, what follows will focus on the quantity of which the mole is the unit, amount of substance.

Official Definitions Are Formal

Let us begin our examination of official definitions with the SI Brochure. We have already seen the current and draft definitions of the mole. Both the current and draft definitions say that the mole is an *amount of substance*. The current definition makes it clear that the mole is related to the number of elementary entities: "The mole ... contains *as many* elementary entities *as* [emphasis added] ...."[5] It does not state what that number is, but it says it is the same as the number of atoms of a reference substance (^{12}C) in a reference mass (0.012 kg). Thus, the current definition is implicitly an operational one: finding out the number of atoms of ^{12}C in 0.012 kg of that substance (which can presumably be done by some sort of

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experiment) gives the number of entities in a mole. The wording of the draft definition does not use phrases like "as many" or otherwise indicate that it is proportional to the number of entities. It does give the number of elementary entities in a mole, albeit in a way that no instructor of introductory chemistry would use (that is, by giving the numerical value of the Avogadro constant). The definitions of units in the new SI are all explicit-constant formulations, which means that the units are defined indirectly by giving the value of a physical constant. Thus, the draft SI Brochure does not say (transparently) that a mole contains exactly 6.022 141 29 $\times$ 10^{23} elementary entities; rather it says "... the numerical value of the Avogadro constant [is] exactly 6.022 141 29 $\times$ 10^{23} when it is expressed in the SI unit mol^{-1}."[2]

The point to notice here is that these definitions are primarily concerned with formal relationships—of the mole to a standard mass of a standard material (in the current SI), to a physical constant (in the new SI), and to the physical quantity *amount of substance* (in both). The observation that educators tend to use other language, by the way, is not in itself a criticism either of the official definitions or of textbook formulations, but a reminder that using a text for one purpose when it was written for another may not produce optimal results.

The SI Brochure is concerned with defining base units, and is less concerned about defining base quantities. For example, it does not define either intuitive quantities such as length or more complex quantities such as thermodynamic temperature. Nor does it really define *amount of substance*, although one might take the following passage to contain a definition:[5]

> *The quantity used by chemists to specify the amount of chemical elements or compounds is now called "amount of substance". Amount of substance is defined to be proportional to the number of specified elementary entities in a sample, the proportionality constant being a universal constant which is the same for all samples.*

The word "defined" in the second quoted sentence is problematic. Is that sentence supposed to be a definition? If so it is inadequate, for stating a proportionality relationship between two quantities does not constitute an adequate definition either formally or pedagogically. (Imagine stating that the energy of a photon is defined to be proportional to its frequency, the proportionality constant being a universal constant—certainly a true statement, but not an adequate definition.) Alternatively, one might take the second sentence to refer to a definition given elsewhere—in an unspecified place. And the first sentence is clearly not an adequate definition, given the circularity of defining *amount of substance* using the word "amount."

Before leaving the subject of official definitions, let us examine the IUPAC Gold Book.[19] The Gold Book serves our purposes because, being a Compendium of Chemical Terminology, it has entries for more terms and quantities, and its definitions are a bit more informative than those of the SI Brochure. Still, looking at a the entries for a few SI units and quantities shows that they are intended not primarily to teach concepts but to illustrate formal relationships. Here are the entries for mass and kilogram:

> **mass**, m: Base quantity in the system of quantities upon which SI is based.
>
> **kilogram**: SI base unit for mass (symbol: kg). The kilogram is equal to the mass of the international prototype of the kilogram.

Clearly, this is not the place to go to learn about the nature of mass.

Let us examine the entry for amount of substance in some detail.[19] My comments appear in italic type in brackets.

> **amount of substance**, n: Base quantity in the system of quantities upon which SI is based. [*Just like mass, so far.*] It is the number of elementary entities divided by the Avogadro constant. [*This tells how to find the quantity in units in which the Avogadro constant is expressed.*] Since it is proportional to the number of entities, the proportionality constant being the reciprocal Avogadro constant [*that is, the reciprocal of the Avogadro constant*] and the same for all substances, it has to be treated almost identically with the number of entities. [*This is rather explanatory; however, "almost identical" is not exactly identical, and the difference is not specified.*] Thus the counted elementary entities must always be specified. ... [*Examples follow distinguishing, for instance, amount of chlorine atoms from amount of chlorine molecules.*] In some derived quantities the words "of substance" are also omitted, e.g. amount concentration, amount fraction. Thus in many cases the name of the base quantity is shortened to amount and to avoid possible confusion with the general meaning of the word the attribute chemical is added. [*Thus IUPAC recognizes possible confusion of this term with the ordinary meaning of amount, and at least offers a word that can enhance specificity.*[20]] The chemical amount is hence the alternative name for amount of substance. [*Chemical amount is a useful suggestion for clarity in communicating with specialists, but it not itself an explanatory term for teaching.*] ... [*Part of the entry dealing with usage in clinical chemistry is omitted from this quotation.*] The quantity had no name prior to 1969 and was simply referred to as the number of moles. [*The assertion that the quantity previously had no name can be taken as true only in an official sense. "Number of moles" is, of course, a name, even though it is not a formally appropriate name because the name of the unit appears in the name of the quantity; still it is a name that chemists used and understood—and continue to use.*]

Official Definitions Equal Scientific Consensus?

The name of the quantity of which the mole is a unit serves as an example of the assertion that SI definitions do not necessarily represent the consensus of scientists. Searching ACS publications for the phrases "amount of substance" and "number of moles" yielded 400 research papers published in ACS journals since the year 2000 that contain the phrase "amount of substance" and 4388 for "number of moles." This would seem to contradict a statement quoted above from the current SI Brochure: "The quantity used by chemists to specify the amount of chemical elements or compounds is now called 'amount of substance'."[5] Whether chemists use the quantity, they rarely seem to call it *amount of substance*. A similar search of the same database, by the way, revealed a strong preference for "Avogadro's number" to the "Avogadro constant" in ACS research publications. This search turned up 1541 research papers published in ACS journals since the year 2000 that contain the phrase "Avogadro constant" or "Avogadro's constant" compared to 5749 that contain "Avogadro's number" or "Avogadro number".[21]

It is clearly desirable to have a special term for the quantity of which the mole is a unit—a term that does not contain the

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word mole. At the same time, it is obvious that use of the official term for this quantity does not represent the consensus of practicing chemists. After all, the data set for this query was research papers published relatively recently—more than a generation after the introduction of *amount of substance* as an SI base unit—in peer-reviewed ACS journals. It represents, by any reasonable assessment, work written and reviewed by experts.

Either Official or Wrong?

And yet there are voices in the educational literature who infer or imply that one does not really know the mole if one does not know *amount of substance*. This line goes back to the time when amount of substance was being proposed as a base unit for inclusion into the SI. From the "Chemical Queries" column of this *Journal* in 1968 comes the question, "Is the mole a number or a weight?" The reply begins:[22]

> *Strictly, neither alternative is appropriate. The mole is the amount of substance containing the same number of molecules (or atoms or radicals or ions or electrons) as there are atoms in exactly 12 g of ^{12}C.*

As if simply stating the term *amount of substance* clears the matter up. To be fair to the authors of the column, they go on to state that in teaching the mole, "It is important to emphasize the amount which is a mole as a number of particles rather than the mass of those particles."[22] It seems to me that this response asserts, in effect, that both number and mass are part of the mole concept. This is consistent with my understanding of the term mole as used by chemists. But the column does not explain the term *amount of substance*; it simply invokes the term (by stating that the mole is a definite amount of substance), and says it is neither a number nor a weight or mass.

A more recent example, from a 2002 article by Furió, Azcona, and Guisasola, asserts[23]

> *The mole concept is wrongly introduced in most chemistry texts, attributing it the meaning of chemical mass and/or number of elementary entities. Such* ***wrong interpretations*** *are also present* ***among prestigious authors and publications*** *[emphases added] and in educators, ...*

This statement seems to treat the mole as if it were a Platonic idea coextensive with its definition: it is what the official definition says it is, and anything else is a wrong interpretation.

What are some of these wrong interpretations? Furió et al. state that their results are in line with findings of Strömdahl, Tullberg, and Lybeck,[24] about a decade earlier. The latter report that only 3 of the 28 Swedish educators in their study identified the mole as the unit of *amount of substance*. Most of the participants selected options that identified it with Avogadro's number (17) or with a formula mass (7). The conclusion of this paper notes that Swedish law requires instruction to be in agreement with the SI. It notes that only a small fraction of the sample of educators interviewed seemed to do so with respect to the mole, and that those who presented the mole otherwise than as an *amount of substance* were unaware that they varied from the SI. The paper continues:[24]

> *But the educator should be aware that this choice has been made on idiosyncratic grounds differing from the* ***prevailing scientific view, expressed by the scientific community through SI*** *[emphasis added].*

Just what the relationship ought to be between scientific consensus and the SI is an interesting question; however, on the mole and *amount of substance*, a serious divergence between the two apparently exists.

■ CONCLUSIONS

A recent article in this *Journal* by Fang, Hart, and Clark notes[25]

> *... while it is necessary that student conceptions of the mole should be consistent with the SI definition, this does not imply that the SI definition is the most effective or appropriate instructional representation of the mole concept.*

Their premise thus seems to be that both the official definition and what expert chemists mean by the mole (and what many chemistry educators already teach about it) are correct. What follows from this premise is that the meaning chemists have previously given the mole is projected onto the term *amount of substance*.[26] These authors present a masterly synthesis of the various aspects of the mole concept, in particular of mass and number. And since *amount of substance* is in many respects a technical term without an adequate official definition, that synthesis does not seriously contradict any widely accepted definition. If the new SI retains *amount of substance* as a base quantity, then let it be explicitly defined along the lines laid out by Fang et al.

My own recommendation is to do away with base quantity *amount of substance*. As a technical term, it does not materially add to understanding the mole. And it is a term that chemists have not embraced, more than four decades after its adoption into the SI. To quote Werner Dierks at the opening of his 1981 paper "Teaching the Mole":[27]

> *Generations of chemists have apparently used the label 'mole' without any difficulties. ... It seems that the definition [that is, its official definition and adoption into SI] has led to difficulties which either did not previously exist or of which we were unaware.*

To which I would add that more than another generation of chemists have used the label mole without being assisted or troubled by the SI definition. There is little prospect of chemists embracing *amount of substance* after the redefinitions of the new SI, so the new SI would be better off without that term.

I close with an admission that this recommendation is inadequate. Having shown that "number of moles" reflects expert usage among chemists and chemical educators and having asserted that as such it is not "wrong" just because it contradicts official definitions, I nevertheless recognize that it is not a logical usage. The principle of distinguishing quantities from units is a sound one. The quantity of which the mole is a unit deserves a better name than "number of moles". Apparently, however, most chemists and chemistry educators do not believe that "amount of substance" serves that purpose.

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Notes

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set out in this essay. Neither the referees nor NTS is responsible for whatever deficiencies remain.

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(6) Note the difference between the Avogadro **constant** and Avogadro's **number**. Officially, the Avogadro constant has dimensions of (amount of substance)$^{-1}$. Its numerical value technically depends on the units in which it is expressed, but those units are invariably mol^{-1}. Avogadro's **number** is the number of entities in 1 mol. Thus, Avogadro's number, which is dimensionless, is the numerical value of the Avogadro **constant**, when the latter is expressed in units of mol^{-1}. None of the chemistry textbooks consulted herein uses the term Avogadro constant.
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