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Are there distinct views of chemistry behind the old and the new definition of mole?

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Abstract

In recent years, the definition of *mole*, the unit of the *amount of substance*, has changed to have the base units of the International System defined by "explicit-constant" formulations. The old definition, by referring explicitly to both mass and elementary units, suggests that the mole is a bridge between the macroscopic and microscopic registers. Conversely, the new definition emphasizes the aspect of counting, referred to any kind of elementary unit. Paradoxically, this results in the disappearance of the notion of substance from the very unit of the quantity *amount of substance*. This change of definition elicited both positive and negative remarks from various authors, in relation to its epistemological, disciplinary, lexical and educational implications. In the present paper, we analyze some of these issues, highlighting the (conflicting) motivations of metrologists and chemists. We argue that the new definition of mole reflects a view of chemistry according to which the microscopic perspective prevails, possibly entailing the loss of reference to the macroscopic register; this could be related with the profound change undergone by the cognitive practices of chemistry along this last century.

Keywords Mole · Amount of substance · Universal constants · Chemical education · Epistemology · Metrology

It is as easy to count atomies as to resolve the propositions of a lover
William Shakespeare, As You Like It

The quantity *amount of substance* and its unit, the *mole*, play a central role in chemistry as they connect the macroscopic realm of substances with the atomic-molecular realm. As substances react with each other in stoichiometric terms (i.e. in terms of constituent particles instead of masses), the *amount of substance* is the conceptual tool that allows setting chemical transformations in stoichiometric terms, through an action of *counting by*

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weighting, thanks to the relationship between the Avogadro constant and the molar mass of each substance.

Despite the long history of this chemical quantity, its foundational character was formally acknowledged only in 1971, when the 14th Conference Générale de Poids et Mesures (CGPM) decided to include the mole in the SI (Système Intèrnationale), at the urging of IUPAP and IUPAC *(Comptes rendus CGPM 1971; SI Brochure Appendix 4 2019)*. This brought the number of base units of the SI to seven.

The definition of the mole approved in 1971 was proposed by the ISO (International Organization for Standardization) and the CIPM (Comité Intérnational des Poids et Mésures) in 1967 and it was confirmed in 1969. This former definition reads as follows:

1. 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".
2. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles. It follows that the molar mass of carbon-12 is exactly 12 grams per mole, M (^{12}C) = 12 g/mol.

In 1980 the CIPM approved the report of the CCU (Comité Consultatif des Unités) which specified that the previous definition refers to unbound atoms of carbon 12, at rest and in their ground state, in order to avoid relativistic effects that might affect the molar mass[1] (SI Brochure 2006).

In recent years, an important conceptual shift has occurred in the SI: the whole system has been re-defined in terms of a set of seven fixed defining constants that are now recognized as "the most fundamental feature of the definition of the entire system of units" (SI Brochure 2019): consequently, the seven base units (and their derived units) of the SI are now derived from these constants.

The decision to derive all units from seven defining constants stemmed from a deep metrological concern, that is clearly stated in the 9th SI brochure (SI Brochure 2019): "To be of any practical use, these units not only have to be defined, but they also have to be realized physically for dissemination". In other words, physical standards are required and need to be realized. The so-called *mise en pratique* (realization of an artifact) may involve the risk of loss, damage or change of the standard reference. On the contrary, the approach based on fixing the universal constants is more abstract; its abstract character allows disconnecting the definition of a unit from its realization, that may occur at any place and at any time. So, the main metrological reasons for changing the theoretical framework of the SI (and, concurrently, the definition of mole) by adopting the universal fundamental constants as the basis for defining the SI basic units, are to be found in the need to disengage from dependence on standard reference artifacts and to build a reference system, stable in time and space.

The new definition of mole proposed according to this more abstract approach reads as follows (SI Brochure 2019)*:*

> 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*

[1] Interestingly, this implies that 0.012 kg of pure carbon-12 in the form of graphite is not exactly 1 mol, if it is in solid form, and at room temperature (Marquardt et al. 2018).

Table 1 Similarities and differences between the 1971 and 2019 definitions of the mole

1971 Definition	2019 Definition
It makes explicit reference to both masses and elementary units	Lack of explicit reference to mass. AoS is identified with a mere count of elementary entities of any kind (a measure of the number of specified elementary entities)
It defines the unit of measurement, not the quantity	It defines both the unit of measurement and the quantity
No explicit mention of Avogadro's constant and its value	It mentions explicitly the value of Avogadro's constant, which is fixed
Need to specify the elementary entities referred to	Need to specify the elementary entities referred to
The molar mass of ^{12}C is defined exactly	The molar mass of ^{12}C is no longer fixed and must be determined experimentally
The mole as a *bridge between the macroscopic and microscopic registers*	The mole as a *particle count*

> *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.

An immediate consequence is that the molar mass of ^{12}C is no longer fixed and must be determined experimentally, so it is subject to change:

> This definition implies the exact relation $N_A = 6.022\ 140\ 76 \times 10^{23}\ mol^{-1}$. Inverting this relation gives an exact expression for the mole in terms of the defining constant N_A: $1\ mol = (6.022\ 140\ 76 \times 10^{23}/N_A)$. The effect of this definition is that *the mole is the amount of substance of a system that contains 6.022 140 76 × 10^{23} specified elementary entities*. The previous definition of the mole fixed the value of the molar mass of carbon 12, $M(^{12}C)$, to be exactly 0.012 kg/mol. *According to the present definition $M(^{12}C)$ is no longer known exactly and must be determined experimentally* (SI Brochure, 2019, italics added).

In summary,[2] a comparison of the 1971 and 2019 mol definitions highlights the aspects reported in Table 1.

The quantity *amount of substance* (AoS) and its unit, the *mole*, have been the object of a long-standing debate among metrologists, chemists and physicists. In the years around 1971, several critical voices raised doubts on the opportunity of introducing the mole into the SI, since the mole and its corresponding quantity were perceived as inherently different from the other quantities and units of the SI. Similarly, the change in the definition of the mole, approved in 2019, was accompanied by a "vigourous debate" (Güttler et al. 2019). Many chemists and metrologists have raised critical remarks on this choice, for different and sometimes opposing reasons (De Bièvre 2015; Emerson 2012; Fang et al. 2015; Gal 2020; Güttler et al. 2019; Johansson 2014; Miller et al. 2011; Marquardt et al. 2017; Schmidt-Rohr 2020; Wolff 2018).

[2] Unless otherwise specified, italics are always introduced by the authors, for highlighting purposes.

In the present paper, we compare and analyze the old and new definition of the mole in relation to the following issues: (i) the reasons of metrology vs. those of chemistry; (ii) the views of chemistry that lie behind the two definitions of mole and (iii) the educational implications of the two definitions.

The reasons of metrology

According to Güttler et al. (2019), the introduction of the mole in the SI "has enabled chemistry to become increasingly integrated into the global metrology infrastructure". On the opposite side, Johansson states that the reasons for including the mole into the SI were sociological, rather than scientific: "From a sociological point of view […] many chemists might have had a feeling that an incorporation of a chemistry unit in the SI system *would enhance the status of chemistry*" (Johansson 2014, italics added). The opportunity of introducing the mole in the SI is a long-standing *vexata quaestio* amongst metrologists, despite the fact that the mole has been part of the SI for more than 50 years. This debate focuses on four main issues:

i) the continuous vs discontinuous character of the AoS;
ii) the fact that the definition of the unit (mol) precedes that of its corresponding quantity (AoS);
iii) the relation between AoS and mass;
iv) the coexistence of quantitative and qualitative aspects in the quantity AoS.

On the first issue, Johansson considers that the introduction of the mole and the AoS into the SI implies an improper mix of continuous and discontinuous quantities:

> "Atoms and molecules are naturally discrete entities, but in the SI system the dimension (or kind-of-quantity) *amount of substance* has nonetheless been forced to conform to a structure that fits only naturally continuous kinds-of-quantity, i.e., quantities such as length, mass, time duration, and so on. This is a mistake, even though an explainable one. *In the SI system, unhappily, the mole is regarded as a unit of the same kind as the metre, the kilogram, and the second*" (Johansson 2011).

Johansson clearly understands the AoS in purely microscopic terms, neglecting its relationship to mass. Schmidt-Rohr (2020) shares a similar concern, as he believes that the 1971 definition of mole "relies on an *outdated continuum view of matter*. By contrast, in chemical practice the mole *can simply be treated as a large number*". This conception will be further discussed later on, in this paper. From a different viewpoint, Güttler et al. (2019) consider that having the mole within the SI is a benefit, as it allows formalizing the dimension of the quantity *amount of substance*, which is thereby distinguished from a pure number (number of entities), i.e. a mere particles' count. Finally, Wolff (2018) discusses the purported ambiguity of the AoS in terms of its double character of continuous quantity and "counting quantity" (discrete quantity). From the metrological point of view, this implies a conflict because continuous quantities (like length, time, etc.) have their own unit, whereas counting quantities lack dimensions (the base unit of a counting quantity is 1).

Moving on to point (ii), AoS is perceived as a "contentious quantity" (Wolff 2018) due to the fact that—unlike basic quantities like length, mass, temperature, time, electric current, or luminous intensity, that are not defined in the SI (only their units are)—the definition of AoS has been incorporated into the most recent definition of mole. In fact, Wolff highlights a peculiarity (or an anomaly) of the 2019 definition: it identifies the mole and concurrently specifies the nature of the corresponding quantity (AoS). This is defined as "a measure of the number of specified elementary entities". Such peculiarity is also remarked by Güttler et al., who think that the new definition of mole.

> "will not help to resolve the awkward historical relationship the mole has had with the quantity of which it is the base unit, amount of substance. This has mainly arisen because, unlike in physical metrology where we first conceive of a quantity and then of its unit, *this happened in reverse for chemistry*" (Güttler et al. 2019).[3]

In fact, the 2019 definition reflects the historical development of these concepts: the mole came first, the AoS was formalized much later.

If the reasons for introducing the mole into the SI were related to both metrological and chemical needs, the drive for the subsequent change of definition of the mole came primarily from metrology:

> "The present (N.B. 1971) definition of the mole is linked to the mass of the International Prototype of the Kilogram (IPK) but m_{IPK} *is not a perfectly stable quantity*. The proposed new SI solves the problem of the IPK by *linking the kilogram to a fixed numerical value of the Planck constant, h*, whose SI unit is kg m^2 s^{-1} (or simply J s because joule is a special name for kg m^2 s^{-2}), and measurements traceable to the SI metre and second, which are already defined in terms of fixed numerical values assigned to two physical constants" (Marquardt et al. 2017).

This leads us to the third metrological reason for revising the definition of mole: the need for an *inherently stable system of units* (Güttler et al. 2019), based on fundamental constants whose numerical values is fixed.[4] The old mole was related to the kilogram, whose mass—defined through the IPK—was not perfectly stable. The re-designed SI, according to Marquardt, solves the problem, as the Kg is no longer tied to the prototype, but rather to the Planck constant. As for the mole, any reference to the kilogram has vanished. In fact, the change of foundation of the SI *dematerializes* all units of measurement, including the mole. From the metrological viewpoint, this is a clear advantage: the independence of the units from material artefacts makes them more universally accessible and applicable. As to the mole, the reliance on a material property of a specific isotope of carbon and the reference to an ensemble of ^{12}C unbound atoms, at rest and in their ground state are both dropped (Marquardt et al. 2018).

The fourth issue of concern to metrologists is the need to qualify the nature of the particles being counted with the mole: "Unlike the other base units, the mole was, and still is, defined by two clauses. The first one defines a number of elementary entities. The second one requires the *identification of the elementary* entities" (Güttler et al. 2019). In fact, an additional note in the SI Brochure reports: 'It is important to give a precise definition of

[3] For a historical account of the origin of the notions of mole and amount of substance, see (Cerruti 1994).

[4] This resolution is not shared by the entire metrological community; in fact, it has been remarked that such constancy may prove illusory or, at the very least, ill-founded on the epistemological level: "When unit definitions are anchored in theories instead of in obviously existing macroscopic magnitudes such as prototypes, meridians, and solar days, then a quite special metrological possibility arises. Since theories are not only about what actually exists and can exist, but also about counterfactual situations that may never exist and may not even possibly exist, *the constancy magnitude that grounds a unit definition can be placed in a non-existing or impossibly existing magnitude*." (Johansson 2014).

the entity involved (as emphasized in the second sentence of the definition of the mole) (SI brochure 2019). Mentioning the mole implies specifying the nature of the substance (or entities) one refers to: "One mole of what?" is the question inextricably linked to the mention of a mole—"The determination of a quantity of substance is made specifically *relative to a [particular] entity"* (De Bièvre 1995). This peculiarity differentiates the AoS from the other base quantities of the SI. In addition, it introduces a "dialectic between quantity and quality" (Turco and Cerruti 2002a) that is problematic for metrology, but it is at the core of chemical epistemology: "The real difference between *amount of substance* and these other quantities is that *amount of substance* is different for different substances, whereas the other quantities are the same, regardless of what substances are measured" (Wolff 2018).

Finally, according to some authors, two further metrological advantages of the 2019 definition of mole are: (i) its explicit mention of the relationship between the mole and the numerical value of the Avogadro constant (Güttler et al. 2019); (ii) the fact that "SI and the metrological system in general would receive the necessary attention among chemists it deserves—and badly needs" (Meinrath 2011). Unfortunately, this last remark seems to have gone unheeded.

The reasons of chemistry

The chemical perspective on the mole and the AoS turns out to be rather different from the purely metrological one. In order to discuss this issue, it is worth comparing the 1971 and the 2019 definitions of mole. Three aspects of the former definition are absent in the most recent one:

i) it makes explicit reference to both masses and elementary entities;
ii) the molar mass of carbon-12 is exactly defined;
iii) the Avogadro number is not explicitly mentioned (Marquardt et al. 2017).

Clearly, behind the 1971 definition is the conception of the mole *as a bridge* between the macroscopic and microscopic registers. The chemical relevance of the notion of mole lies precisely in this bridging character between two distinct realms:

> "the role played by the quantity *amount of substance* in laws of nature is that of a *mediator between macroscopic measurements and microscopic measurements* describing these chemical and thermodynamic phenomena in terms of molecular interactions. […] On the macroscopic level the description of the phenomena is presented in terms of macroscopically continuous quantities like mass, volume, pressure, and temperature. *An explanation of the macroscopic relations is offered in terms of microscopic entities (atoms, molecules), which are typically too small and too numerous to count*" (Wolff 2018).

Along a similar line, the metrologists Güttler et al. (2019) remark that: "The mole is important in chemistry because it recognizes that atoms and molecules react together on an *amount of substan*ce basis and not on a mass basis". The relation between chemical reactivity and AoS is a fundamental one to chemistry**:** "the amount of substance expresses the reactivity of matter by freely indicating the stoichiometry of the physical system to which it refers" (Turco and Cerruti 2002a, our translation). This epistemic posture has its roots in the history of chemistry and the microscopic hypotheses that marked its birth as a science:

"The *amount of substance* allows a quantitative formulation of the law of multiple proportions due to Dalton and Avogadro" (Marquardt et al. 2017). Most relevantly, Marquardt et al. also underline that any chemical (stoichiometric) equation is subjected to a "macroscopic and a microscopic (particulate) interpretation" thanks to the introduction of the base quantity AoS, which "*reflects both views*". The history of chemistry reminds us that chemists measured the AoS of most substances precisely by making these substances react with each other. In doing so, they performed "in the material world that operation of *two-way correspondence* between the microscopic components of macroscopic systems indicated by the definition of mole" (Turco and Cerruti 2002a, our translation).

Finally, an authoritative remark on the meaning of the mole (and the Avogadro constant) in relation to the chemical behaviour of substances and the connection between *macroscopic and microscopic* realms, comes from none other than Max Planck:

> "The physical forces, gravity, electric and magnetic attractions or repulsions, cohesion, act in continuous way; *the chemical forces, on the contrary, by quanta*. This law would be connected with that which allows masses in physics to act each one on the other in whatever quantity, *while in chemistry they can act only in sharply defined proportions, variable in discontinuos manner*" (Planck 1912).

In summary, the notions of mole and AoS are crucial to chemistry insofar as they allow the macroscopic and microscopic realms to be linked, thus enabling *quantitative* interpretations of the observed chemical behaviours to be provided in terms of microscopic particles and their interactions.

The mole and the amount of substance: a mass, a particles' count or a bridge between them?

The distinction of the AoS from mass or a particle count has been addressed by several discussions, in the metrological and chemical literature and in the frame of the CCU meetings. In 1969, the then president of CCU De Boer, while introducing the discussion on the subject "*Should we adopt an SI unit of amount of substance?*" stated that "most physicists perhaps do not realize with sufficient exactitude the *physical meaning of mole*"; he also added that it was unthinkable to measure the quantity of substance in units of mass (CCU 1969, our translation). De Boer clearly had in mind the reasons of chemistry and those of metrology, as well as the need to keep them together. In the same context, the English physical chemist McGlashan remarked that:

> "the mole, which draws its origin from the old concept of chemical equivalents [...] cannot be replaced either by a number or a mass [...]. *It would be particularly nefarious to lead back to a pure number the quantity to which the mole corresponds*. Indeed, for more than a century, chemists have treated the mole as an independent unit" (CCU 1969, our translation).

Strangely enough, this is precisely what the most recent definition of mole seems to accomplish: "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 […] The *amount of substance*, symbol n, of a system is a *measure of the number of specified elementary entities*" (SI Brochure 2019). The new definition emphasizes the aspect of counting, referred to almost any elementary entity. But, de facto, it goes even further: it identifies the mole with a mere particle count

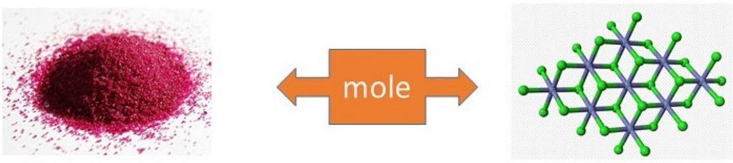

Fig. 1 Relationship of the mole with the macroscopic and microscopic realms

(a *measure of the number of specified elementary entities*). This is a direct consequence of the lack of any explicit reference to mass, that was avoided expressly for metrological reasons. In fact, referring to both levels is problematic to metrologists; however, *this duality is essential to chemistry.*[5]

Thereby, a situation of *epistemic conflict* between two disciplines is being produced: the absence of reference to mass is the main metrological reason for having a new definition of mole. However, the loss of that reference empties the mole and the AoS of their deeper chemical significance, which is to *act as a mediator* between the macroscopic and microscopic realms (hence their relation to both mass and particles' count). Such interdisciplinary conflict was not apparent in the former definition, where the aspect of counting (particles) was strictly related with the action of measuring a macroscopic quantity (mass, in the case of atomic or molecular substances; charge in the case of electrons; etc.). Turco and Cerruti remind us that the amount of substance.

> "takes on *one of the most characteristic features of chemists' epistemology, the continuous and contextual reference to two different levels of reality*, the macroscopic and the microscopic. In fact, the first part of the *[1971]* definition, speaking of a mass of 12 g, firmly anchors the mole to a world of macroscopic corpuscles, manipulable with flasks and filters, while the second part refers back to 'objects' of the subatomic, atomic, and molecular worlds, to be described otherwise as mere stoichiometric references" (Turco and Cerruti 2002a, our translation).

From the chemical viewpoint, the mole is a *two-faceted concept* aimed at connecting two distinct levels of reality: its place is precisely *in between* these levels (Fig. 1). Losing (or giving up) one of these two dimensions affects the meaning of this concept, as it flattens it out to a unidimensional notion, and disregards its historical development.

Gorin (1994) brings an additional argument to demonstrate why the AoS cannot be reduced to a number (i.e. a count)*:* "chemical amount is determined from the stoichiometry of chemical reactions. The relative number of atoms involved in the reaction may be deduced from such measurements, but one cannot proceed in the opposite sense, because, as was stated at the outset, *there is no direct experimental procedure by which atoms can be enumerated*". In other words, AoS is a conceptual tool that allows *counting by weighting*. If the aspect of weighing is put aside, the concept of mole changes its nature.

[5] Although this statement refers to the mole, chemistry offers other examples of 'dual concepts', e.g. the notions of element, substance, entropy, etc. In most cases, duality stems from the fact that chemical descriptions rely on distinct registers (macroscopic and microscopic descriptions). This is a well-known problem that has been thoroughly discussed in chemical education (see, for instance, the work of Alex Johnstone and the so-called Johnstone triangle), as it may result in severe misconceptions. From the epistemic viewpoint, several contributions on the duality of specific chemical notions are available in the literature, but a general reflection on the role of dual concepts in chemistry probably deserves further developement.

While remarking that the new definition of the mole misses the connection to mass, Wolff (2018) stresses the fact that the AoS "is more than a mere counting quantity, because it can only be applied to samples of the same chemical substance, which is a constraint not placed on counts of entities in general". In saying so, he criticizes the new definition of mole, not just because "the mole is defined as a pure number of elementary entities" but also because "the definition gives no particular indication of where that number comes from". To this regard, Turco and Cerruti recall that before the concept of mole there is that of *equivalence between moles of different substances.* It is precisely to this equivalence that the definition of mole refers to, and not to any number (Turco and Cerruti 2002a, our translation).

In summary, the transition from the old to the new definition of mole – examined from the chemical viewpoint – entails the loss of explicit reference to molar mass and the enhancement of the counting character. What is desirable and beneficial on the metrological level, turns out paradoxical on the chemical level as it results – de facto—in the disappearance of the substance from the very unit of the amount of substance. A substance is a tangible entity, that can be weighted, stored in a container, can exhibit several macroscopic properties according to which we identify it as a substance, and can also (but not exclusively) be described in microscopic terms. Nevertheless, this view is not shared by all chemists. When Schmidt-Rohr (2020) states that "a substance essentially equals the molecules of which it consists, and therefore, *amount of substance* is equal to the *number of molecules"*, he takes a reductionist, microstructuralist stance that corresponds to a strongly realist conception of the microscopic realm. From our point of view, this position has some obvious limitations: (i) it does not take into account the complexity of any material system, which is more than the sum of its components, at least due to the relationships that bind these components; (ii) it promotes an ahistorical view of chemistry; (iii) it does not highlight the (ontologic and epistemic) distinction between macroscopic and microscopic realms. This latter aspect is problematic from the educational viewpoint: in fact, only the reference to a macroscopic dimension (the dimension of manipulation) justifies the microscopic description in terms of particles (i.e. modelling). Without a macro reference, the microscopic world would lose its *raison d'être* as, within the chemistry domain, it serves precisely to interpret the phenomena occurring in the macroscopic realm.

Which name for the quantity of which the mole is the unit?

The mole is the unit of the AoS. The definition of mole specifies that this quantity is a measure of the number of specified elementary entities: these may be atoms, molecules, ions, electrons or "any other particle or specified group of particles". Albeit the notions of mole and AoS take their origin in the need for quantifying the relationship between the reactants of a chemical transformation, these notions have been extended to entities other than atoms and molecules. In doing so, the amount of substance has disengaged from the notion of substance. Schmidt-Rohr (2020) remarks that: "there is neither a conventional "electron substance" nor a "hydronium substance". Therefore, the substance-based definition of the mole, which works fine for common pure substances like tin, water, or oxygen gas, fails in these important cases". A similar remark comes from Baransky (2012): "The term substance is applicable to characterization of elements and chemical compounds, that is, the type of matter with a uniform, well-defined composition (even at microscopic level). […]. A mole of electrons, also named the Faraday constant, amounts to the charge of 96,485 coulombs, and it cannot be labelled substance". Hence, in several cases, the term *amount of substance* is not appropriate.

Here we deal with a lexical problem, strictly entangled with a conceptual aspect: is it still acceptable to call *amount of substance* the quantity of which the mol is the unit?

On August 26th 2009, the CCU recommended that "The greatest effort should be made to change the name of the ISQ base quantity *amount of substance* at the same time that a new definition of the mole is approved" (Marquardt et al. 2017). The motion was approved unanimously by the IUPAC Executive Committee.

To the best of our knowledge, the question has not yet been solved, although this issue is extensively discussed in the literature (De Bièvre 1995 and 2015; Giunta 2016; Gorin 1994; Cerruti 2003 and 1984; Schmidt-Rohr 2020). Several proposals have been made, often aligned with the new definition of mole. For example, Johansson (2011) suggests to rename the *amount of substance* as *number of elementary entities* or simply *entities*. According to Baranski (2012) the *amount of substance* might be replaced by *collection or quantity of microentities*. Both proposals clearly reduce this quantity to a mere particle count, no matter what kind these particles are. In fact, Baranski (2012) goes even further by suggesting that: "Mole is a term similar to dozen or score. These units are undoubtedly useful if the counted objects are identical, such as unused pencils, matches, nuclides, or electrons". These proposals lead to the consequence that the chemical specificity would depart from this quantity as they extend its applicability to any particle and, concurrently, they neglect the character of mediator between distinct levels of reality that is typical of the notion of mole. Their perspective is entirely microscopic and abstract. Reference to the macroscopic world of substances is no longer perceived as necessary.

A proposal that highlights the peculiar chemical significance of this quantity comes from Leonard (2007), who argues that the name for the base quantity should be *chemical amount*. This position is also supported by Giunta (2016) and Gorin (1982). Marquardt et al. (2017) remark that the term *chemical amount* has appeared as the alternative name for *amount of substance* in the IUPAC Green Book since 1993 (IUPAC Green book 1993).

Interestingly, further lexical issues become apparent when one takes into account the different translations of the term *amount of substance*. A thorough comparative linguistic analysis can be found in Cerruti (1984 and 2003). The most striking divergence pertains to the French language, where the quantity measured by the mol is designated as *quantitè de matière*: here, the *substance* is replaced by a more generic *matter*, that has completely different chemical implications as compared to substance. Another linguistic issue pertains to the designation of the elementary entities that are enumerated in the mole: according to Cerruti (2003), the best expression is the German one. The term *Einzelteilchen* – single or separated or individual particle—is more appropriate as compared to entities or elementary entities because it suggests isolation, identifiability rather than elementarity. As for the quantity whereof the mol is the unit, it is worth remembering that the English term *amount of substance* was derived from the German term *Stoffmenge* introduced by Stille (Güttler et al. 2019).

Which views of chemistry lie behind the two definitions of mole? Which are their educational implications, if any?

The conceptual shift that accompanies the change of definition of the mole lies basically in conceiving the mole as a count, from a completely microscopic perspective, rather than as a mediator between macroscopic and microscopic realms (with reference, respectively, to the mass and to the Avogadro constant). This shift has both disciplinary and educational implications. As the notion of mole has often been reported to be perceived as a difficult notion by student (Furio et al. 2002), one may wonder which definition is preferable from the educational viewpoint.

According to some authors, the conception of the mole as a count "should help to eliminate confusion between the quantities of amount of substance and mass"; at the same time, the new definition may cause even more confusion "when it comes to distinguishing counting quantities from amount of substance" (Güttler et al. 2019). Güttler et al. are clearly concerned by the danger of confusing two quantities that are, in fact, distinct (mass and AoS), and are measured by distinct units (gram and mol). Another attitude that is quite popular among those who support the view of the mole as a count is comparing the mole to a dozen: "The recent revision has moved the mole from a mass-based closer to a number-based definition. In this framework, the mole is a number unit analogous to dozen or percent. […] These unifying equalities will make it easier to learn and teach chemistry" (Schmidt-Rohr 2020). An argument against assimilating the mole to the dozen is brought by Brown (2023): he remarks that the mole refers to *elementary entities* and the AoS is "the property of a system". According to this author, "*Elementary entities* restricts the things that may be described to those that could take part in stoichiometric chemical reactions together and are sufficiently elementary that it is possible to define an identical set for the purpose of such a reaction". As for the reference to a system, it "implies the elementary entities considered are located in close enough vicinity such that they could, in theory, react or interact with each other stoichiometrically". So, the quantity AoS does not refer to a bunch of particles, but to a *system of particles* that are related with each other in a well-defined chemical context. Schmidt-Rohr goes even further, as he seems to put into questions the very necessity of the quantity AoS:

> "We propose that even for pure substances, the concept of AoS *is based on an illusion:* If our eyes could resolve water molecules, *we would view water as a collection of molecules and immediately recognize that the number of water molecules is their 'amount'*. This lack of recognition of the atomistic make-up of substances is often called a macroscopic or, more accurately, continuum view; […] in other words, *amount of substance* is apparently *based on the continuum illusion*" (Schmidt-Rohr 2020).

Here we have a completely reversed perspective, with the molecular-atomic (modelling) realm taking the place of the phenomenological world. According to this view, a substance is reduced to the (static) set of its molecules and the reality of substance itself is replaced by that of its microscopic components. In fact, these statements points to a dematerialisation of the mole. The AoS, thought as particle count, overlooks the fact that there is no direct mean to count those particles: one has always to rely on other quantities, like mass or—in the case of electrons or photons—electric currents, energies, etc.

According to Schmidt-Rohr, conceiving the mole as a count would solve both conceptual and educational problems: "Consistently presenting the mole as a number, rather than first introducing it as the unit of a vaguely defined quantity but later treating it *unofficially* as 6.022×10^{23}, will greatly reduce confusion when students learn about the mole" (Schmidt-Rohr 2020). It seems to us that this position shows strong weaknesses from both the epistemic and the educational viewpoint. Schmidt-Rohr seems to forget that any theory has its counterpart in the real world: nobody will ever be asked to weight 6.022×10^{23} molecules of a substance. In the real world, we can weight masses. This immediately raises two questions: which mass corresponds to the number of molecules I need to manipulate in my experiment? Why does 6.022×10^{23} molecules of, let's say, ^{12}C correspond precisely to a mass of 12 g? Put in other terms, Schmidt-Rohr's argument overlooks the dialectic relationship between material realm, theory and models that is at the basis of the scientific approach to reality.

Apart from these educational concerns, it seems to us that the widely (and somehow passive) acceptance of the new definition of mole by most part of the chemical community reflects a deep change in how chemists conceive their own discipline and disciplinary practice.

The transition from the former to the most recent definition of mole entails: (i) a loss of reference to mass (hence to the macroscopic level of manipulation and continuum quantities); (ii) an emphasis put on the microscopic level, that is thought of independently from the empirical realm; (iii) an emphasis put on the aspect of counting.

In this regard, Cerruti (1984, p.52) denounces a cultural pressure aimed at identifying the mole with a number. Our thesis is that the impressive evolution of the cognitive practices of chemistry, which has occurred in recent decades, has inevitably led to an increasingly introspective exploration of the microscopic world to which chemistry refers. Chemical hermeneutical practice allows reasoning in terms of shared electron pairs, single molecules, electrons jumping from one energy state to another, orbitals, proton translocations, etc. The interpretive power of chemistry lies precisely in this ever-increasing ability to explain phenomena with increasingly advanced microscopic models. Clearly, the need to apply stoichiometric reasoning to these entities is real. However, chemists' hermeneutical habits raise two questions and highlights a double risk, at the epistemological level. The questions are: Does reference to any particle authorize the reduction of the mole to a count? Would such a reduction not cause the quantity AoS to lose its conceptual utility? The two risks are: (i) to reify the microscopic world, by treating it as if it had the same prerogatives as the macroscopic and experiential world; (ii) to lose sight of the fact that the microscopic description of the world finds its *raison d'être* in the phenomenal world. If this aspect is overlooked, microscopic descriptions take on an improper autonomy that can lead to inappropriate conclusions (such as, for example, the outcome of a theoretical chemistry calculation unsupported by experimental verification).

This last attitude is well exemplified by Johansson, when he states that.

> "In the connection rule introduced, n mole(X) = $(A_N\ N)(X)$, the right hand side is *ontologically more basic* than the left hand side, *since it is discrete entities or samples of such that are what modern chemistry is about*" (Johansson, 2014).

No doubt, chemical explanations rely on microscopic discrete entities (albeit, not exclusively). Nevertheless, the assignment of a greater ontological weight to the particle realm as compared to the macroscopic world is problematic, as long as the goal of chemistry is still to offer an interpretation of the material world as we experience it: only in this perspective, the recourse to the particle realm is justified. In this regard, the inter-relation between phenomenal and microscopic levels is especially relevant in chemical education: whenever it is neglected or overlooked, it results in serious misconceptions.

Conclusions

The change in the definition of the mole was dictated by the needs of metrology, but it does not fully meet the epistemic specificities of chemistry and carries the risk of overlooking or taking for granted the dialectic relationship between empirical realm, theory and models that is at the basis of any scientific approach to reality. Nevertheless, the fact that such a change has gone unnoticed to most chemistry practitioners may be a reflection of the profound change of cognitive practices that has occurred over several decades. On the educational level, the change raises issues, especially with regard to question of the relationship between physical realm and its interpretive models.

In conclusion, we'd like to quote an exhortation expressed by Turco and Cerruti long ago, but more valid than ever: "Certainly we cannot say that the amount of substance and the mass have made a triumphal entrance into the metrological citadel, however they have been at the top of the International System of Units for more than three decades, a position of eminence *that should bring chemists back to their cultural responsibilities*" (Turco and Cerruti 2002b, our translation).

Although it has been some time since Turco and Cerruti made this reflection, the question of whether or not chemists are fully aware of their cultural responsibilities remains open.

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