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ABOUT MOLES AND “AMOUNT OF SUBSTANCE”...

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Abstract : Comments about the words used to define the mole and the “amount of substance”.

Résumé : Commentaires à propos des termes employés pour définir la mole et la “quantité de matière”.

Many books mention the legal definition of the mole (I.U.P.A.C. ; in France : C.G.P.M. and Decree n° 75-1200 from 4.12.1975) :

> • The mole (symbol mol) is the legal measurement unit for amount of substance : “The mole is the amount of substance of a system which contains as much elementary entities as they are atoms in 0,012 kilogram of 12 carbon. When one uses the mole, entities must be specified and may be atoms, molecules, ions, electrons, other particles or specified groups of such particles”.

Then if one search in this a definition of the amount of substance, it seems that it does exist only on a relative way : the “definition” of the mole is supposed to “define” at the same time intuitively the amount of substance which it is used to measure.

Although not redhibitory, such a situation, easily source of contradiction, must be considered carefully :

> • first the “amount of substance” (or “amount of matter”) of a system is proportional to the number of specific elementary material entities which this system contains (therefore, the kind of entities must be specified, otherwise one does not know what is counted) ;
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> • after, and only after, the mole is the amount of substance of a system which contains as much elementary entities as there are atoms in 12 g of 12 carbon (and that defines the unit mole by setting the coefficient of proportionality).

Then, is there the same amount of substance in one mole of iron atoms and in one mole of copper atoms ? Yes if one defines the “substance” as being “atoms” since there are as many atoms of iron in one mole of iron atoms as atoms of copper in one mole of copper atoms. No if one defines the “substance” as being “elementary particles” (protons, neutrons, electrons...) since there is not the same quantity of these particles in one mole of iron atoms and in one mole of copper atoms.

In reality the expression “amount of substance” merely is incomplete since there exist many different kinds of “substance” (“iron substance”, “copper substance”...). The specification of the chemical element is likewise insufficient : one must avoid to use expressions as “amount of sulphur” without specifying if it concerns the amount of sulphur atoms or the amount of octasulphur molecules.

Indeed in these conditions, is it possible to say that there exists a difference between the concepts of “amount of iron atoms” and “number of iron atoms” ? Certainly not, otherwise one could build like that many new concepts ; for example a concept of “amount of length” :

> • the “amount of length” between two points is proportional to the distance between these points
> • the league is the “amount of length” between two points the distance of which is 4,445 km.

Then it appears that such "definitions" define only a new unit to measure the distances, and not a new concept.

> ◊ remark : this is not away from the definition of a new metric, with a "coefficient of proportionality" depending on the points considered, which may correspond to a non flat Riemann space and therefore to a new physical concept ; but if one changes only the mathematical description of a same physical space by multiplying the metric by a constant coefficient of proportionality, there is no new physical concept.

Likewise the "amount of iron atoms" is not a different notion as the number of iron atoms, but only a different way to count them (otherwise this would come to consider that electric current is not the same physical concept according as it is measured for example in amperes or in milliamperes).

Indeed, an expression like "one mole of iron" has no more sense than "one pair of iron" or "one million of iron", but on the contrary one can say "one mole of iron atoms" as "one pair of iron atoms" or "one million of iron atoms". Therefore "one mole" is to $\mathcal{N}_A \approx 6{,}022.10^{23}$ what "one pair" is to 2, or "one million" to 10^6. One can furthermore think to use the mole to count other things than "elementary constituents" of chemistry : one mole of letters ($\mathcal{N}_A$ letters), and even abstract things : one mole of ideas ($\mathcal{N}_A$ ideas). The fact that the mole has been imagined at the outset with the object of counting material entities constitutes therefore nothing but a particular case[1].

Therefore it seems desirable to attempt to improve its wording ; for example :

- systematically forsake the expression "amount of substance" on behalf of expressions as "number of molecules (or ions, atoms, elementary particles...)".

- modify the definition of the mole : "the mole is a cardinal number, used in practice to count the numbers of molecules (or ions, atoms, elementary particles...), equal to the number of atoms that there are in 0,012 kilogram of 12 carbon" ; thus in practice $\mathcal{N}_A \approx 6{,}022137.10^{23}$.

- do not class anymore the mole among the basic units of the international system, but with the annex symbols for multiples.

> ◊ remark : in this way, the present notation $\mathcal{N}_A \approx 6{,}022.10^{23}\ \text{mol}^{-1}$ becomes absurd in that it would correspond to : $\mathcal{N}_A = 1$; one would have to use on the contrary $\mathcal{N}_A = 1\ \text{mol} \approx 6{,}022.10^{23}$ (similar to the use, for charges units, of the faraday $\mathcal{F} = 1\ \mathcal{F} \approx 96500$ C) ; moreover, the use of some constants would be simplified, for example the perfect gas constant would become identical to the Boltzmann constant : $R = k_B \approx 8{,}31\ \text{J.K}^{-1}.\text{mol}^{-1} \approx 1{,}34.10^{-23}\ \text{J.K}^{-1}$; the atomic mass ($12\ \text{g.mol}^{-1} = 12$ a.m.u. $\approx 1{,}99.10^{-23}$ g) would be used in place of the molar mass (mass of a mole : 12 g) ; and so on...

This would lead not to look as if one gives arbitrarily to a number of particular entities the appellation "substance" (after all the mass, through the relation $E = mc^2$, represents the "amount of material energy" and is therefore quite as much connected to the "amount of substance" ; the volume as well).

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[1] More precisely, the first chemists confronted with the serious measurement of quantities reach the idea of a proportionality with respect to a "number of elementary entities", but the notion of atoms was still "blurred" and the proportionality coefficient (Avogadro number) was unknown, from which a definition of the mole in order to be able to refer to mass measurements. When afterwards, this number became known, this was with a weak precision and it were rather unwelcome to annihilate the beginning of "good practice" for mole counting which became established. Is it still the case now ?

But one can even go further and propose to use the mole to count various units : one mole of metres ($\mathcal{N}_A$ metres, unit of length as well as kilometre ; one could say as well one molemetre and use the symbol molm), one mole of grams (unit of mass as well as milligram), one mole of moles ("counting unit" as well as milliard of milliards).

Therefore, one is brought to think that it may be blundering to use this multiple "mole", which is numerically not known exactly, and which is not a round sum in the decimal system, when there exists in the international system the near multiple "yotta" (10^{24}, symbol Y). This situation is rather similar to the use of the annex pressure unit "atmosphere" (which use as a reference as been largely left out to the advantage of the annex unit "bar", which has at least the merit to be a round sum in decimal system).

Of course, the present definition has for chemistry (according to the initial ideas which induced this definition) the advantage to give simple relations with masses.

But therefore inversely, how not to think to the heteroclite story of the mass unit, which basic name "kilogram" contains a prefix ("kilo", because one has been unable to realize precisely enough a standard for one gram), and which beautiful standard of iridized platinum looks like a few obsolete ?

One solution would be (for example) to choose the mass unit as $\frac{1}{12}$ of the mass of $6{,}022137.10^{23}$ atoms of 12 carbon (exactly), in the same way as one used for the speed of light and the length unit. Of course, even if one do not take advantage of this to round to 10^{24} atoms (this would bring many conversions problems), one could take advantage of this to change the unit name for a basic name without multiplicative prefix.

> ◊ remark : I am rather hopeless ; in an time when it is not only difficult to cause renouncement of units as "calorie" for benefit of the international energy unit "joule", but when it is also difficult to cause overall acceptance of the kilogram unit, it is tricky to scheme such an approach.

It seems however that, at the present time, some physicists do consider problems of this kind [1]. I feel they are right when they propose a definition for mass unit based upon a redefinition of the fundamental Planck constant (h) rather than upon the Avogadro number. As for the speed of light in vacuum (c), an exact value defining h would automatically rely (through the relations $h\nu = E = mc^2$) the time, energy and mass units, while letting possibility to keep the values at the present time admitted. This would be elsewhere fully compatible with the modification I suggest for the interpretation of the "mole".

References :

[1] "Redefinition of the kilogram: a decision whose time has come", I. Mills et coll., Metrologia **42** (2005), p 71.