

The mole *is* an Avogadro number of entities.

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The University of Akron, June 4th, 2014

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Most people seem to agree that the mole is (and should be, as in the current definition) an Avogadro number of entities, where the Avogadro number is the ratio of the gram to the “atomic mass unit.” Historically, the latter has been defined as the mass of a hydrogen atom, then later as 1/16th the mass of an atom of oxygen (or, specifically, oxygen 16), and currently as 1/12th the mass of an atom of carbon 12. [The latter is properly called the dalton, Da, since the term “unified atomic mass unit” cannot sensibly take SI prefixes.] Most people (with the notable explicit exception of the architects of the New SI—and, implicitly, those who have accepted their proposals) agree that it follows that one mole of a given substance has an associated mass that, when expressed in grams, has a numerical value exactly equal to the relative entity mass (“atomic, molecular, formula weight”) of that substance. This is, *and always has been*, the traditional mole concept.

Currently, the gram-to-dalton mass-unit ratio is an inexactly known number determined by experiment. Some people would prefer g/Da to be a specified integer—this can be achieved in one of only two ways: (i) if the carbon-12-based dalton is retained, then the kilogram must be redefined as a specified integer multiple of the carbon-12 atomic mass, or (ii) if the kilogram is not based on carbon 12 (e.g., a “fixed-*h*” kilogram), then the dalton must be redefined exactly in terms of the kilogram—i.e., one kilogram divided by a specified integer. In either case, g/Da = (0.001 kg)/Da is then an exact integer. Case (ii) would decouple the dalton from the carbon-12 reference mass used for cataloguing, to very high precision, directly measured nuclidic mass ratios, $12 \{m_a(X)/m_a(^{12}\text{C})\}$, which, being dimensionless, do not require a unit. It would not affect the values of relative entity masses, $M_r(X) = m_a(X)/\text{Da}$, within the precision used in stoichiometry—with the exception of $M(^{12}\text{C})$, which would differ from *exactly* 12 g mol⁻¹ by an inexactly known term of order 10⁻⁹ or less.

Defining the mole as an exact Avogadro number of entities is similar to the definition of the second, written as:

$$1 \text{ s} = (9\,192\,631\,770) \times T(\text{Cs}), \text{ exactly}$$

i.e., a specified integer times the duration of one cycle of the caesium-atom radiation.

[Note that this is not: $1 \text{ s} = (9\,192\,631\,770) \times 1 = 9\,192\,631\,770$. The symbol “ $T(\text{Cs})$ ” represents a “reference constant,” the duration of one caesium radiation cycle, not the number 1.]

Also, if the coulomb were to be redefined in terms of the elementary charge (rather than the other way around, as in the CCU proposal), this would be written (for example) as:

$$1 \text{ C} = (6.241\,509\,343 \times 10^{18}) \times e, \text{ exactly}$$

i.e., a specified integer times one elementary charge.

[Note that this is not: $1 \text{ C} = (6.241\,509\,343 \times 10^{18}) \times 1 = 6.241\,509\,343 \times 10^{18}$. The symbol “ e ” represents a “reference constant,” one elementary charge, not the number 1.]

Defining the mole as an exact Avogadro number of entities would be written (for example) as:

$$1 \text{ mol} = (6.022\,141\,29 \times 10^{23}) \times \text{ent}, \text{ exactly}$$

i.e., a specified integer times one entity.

[Note that this is not: $1 \text{ mol} = (6.022\,141\,29 \times 10^{23}) \times 1 = 6.022\,141\,29 \times 10^{23}$. The symbol “ent” represents a “reference constant,” one entity, not the number 1.]

If the number of entities of the substance were not equal to the Avogadro number, then we would have a physical quantity that was either a proper fraction or a multiple of one mole. For example, if we had a sample of water consisting of approximately 3.011×10^{23} entities (water molecules, in this case), we would have a physical quantity, $n(\text{H}_2\text{O}) = 0.5 \text{ mol}$, to the indicated precision. If we had approximately 1.807×10^{24} water molecules, the physical quantity would be about $n(\text{H}_2\text{O}) = 3.0 \text{ mol}$. The question then becomes, “What do we call this physical quantity whose macroscopic unit is the mole?” In most textbooks and on-line tutorials, this quantity is simply called the “number of moles” of the specified substance or sometimes just “moles” of the substance. In the above examples, we would typically see: “number of moles of $\text{H}_2\text{O} = 0.5 \text{ mol H}_2\text{O}$ ” or “moles of $\text{H}_2\text{O} = 3.0 \text{ mol H}_2\text{O}$.” This, of course, is unadulterated

gibberish. [There is a legitimate definition of the “number of moles”: $n(X)/\text{mol}$. In the above cases, the *number* of moles is approximately 0.5 and 3.0, respectively. Adding a “label” (such as H_2O) confusingly suggests that the mole is a different unit for each different substance, which, of course, it is not.]

The CIAAW/ACD proposal would call the physical quantity “number of entities.” In the above examples, we would then have: “the number of entities of water, $n(\text{H}_2\text{O}) = 0.5 \text{ mol}$ ” or perhaps “the number of water molecules, $n(\text{H}_2\text{O}) = 3.0 \text{ mol}$.” But the *number* of water molecules (entities) is, respectively, $N(\text{H}_2\text{O}) = 3.011 \times 10^{23}$ and $N(\text{H}_2\text{O}) = 1.807 \times 10^{24}$, not $n(\text{H}_2\text{O}) = 3.011 \times 10^{23} \text{ ent}$ and $n(\text{H}_2\text{O}) = 1.807 \times 10^{24} \text{ ent}$. In other words, “number of entities” is the name of the (dimensionless) quantity represented by $N(X)$. If we want to use the “mole” as a “unit” for “number of entities,” then the mole must be defined as the Avogadro *number*, g/Da, not an Avogadro number of *entities*, (g/Da) ent. The mole would then be a convenient reference number so that we could express $N(X)$ in multiples (or submultiples) of one mole (the “chemist’s dozen”):

$$N(X) = N(X)/(\text{g/Da}) \text{ mol} = N_r(X) \text{ mol} \quad (1)$$

where $N_r(X)$ is the “relative number of entities.” The symbol $n(X)$ would not appear. And the Avogadro constant, *defined* as $N(X)/n(X)$, would be nonexistent.

On the other hand, we could give $n(X)$ a special name, such as: “enplethy.” In the above examples, “the enplethy of water, $n(\text{H}_2\text{O}) = 0.5 \text{ mol}$,” etc. Please insert any other name for the physical quantity whose macroscopic unit is the mole and see if it sounds as artificial as “enplethy.” Personally, I have no problem with “amount”—with the understanding that the formal technical name is “chemical amount,” where the adjective can be omitted, just as “electric” is usually omitted before “current.” [For those who are concerned that subatomic particles and photons, for example, are not “chemicals,” please take the adjective to imply “physiochemical.”] In the above examples, we would say that the “amount of water is $n(\text{H}_2\text{O}) = 0.5 \text{ mol}$ ” or the “amount of water is $n(\text{H}_2\text{O}) = 3.0 \text{ mol}$.” And this sounds perfectly natural, while being technically correct.

The relationship between $n(X)$ and $N(X)$ is simply:

$$n(X) = N(X) \text{ ent} \quad (2)$$

—the (chemical) amount of a specified substance is an aggregate of $N(X)$ entities. The space before “ent” indicates that one entity, being the smallest (non-trivial) amount of any substance, is the appropriate “natural” atomic-scale *unit* for chemical amount, paralleling the dalton for mass: $g = (g/\text{Da}) \text{ Da}$ and $\text{mol} = (g/\text{Da}) \text{ ent}$. Equation (2) is obviously compatible with “the mole is an Avogadro number of entities,” as seen by setting $N(X) = g/\text{Da}$. One entity (ent) is not only the reference constant for defining the mole, it is also the reference constant linking $n(X)$ and $N(X)$, and the atomic-scale unit of chemical amount. Note that the dimension of ent is chemical amount. By contrast, the conventional SI constant linking $n(X)$ and $N(X)$ is the “Avogadro constant,” *defined* as $N_A = N(X)/n(X)$, with the dimension of *reciprocal chemical amount*. The Avogadro constant is not well understood—often being confused with the dimensionless Avogadro number—and this is one of the main sources of the well-known confusion permeating this subject. From Equation (2), when $N(X) = 1$, $n(X) = 1 \text{ ent}$, so the Avogadro constant is (*always*): $N_A = 1 \text{ ent}^{-1}$ (one per entity), independent of macroscopic units.

The relationships between “number of entities,” $N(X)$, “substance mass,” $m(X)$, and “chemical amount,” $n(X)$, are very straightforward:

$$N(X)/(g/\text{Da}) = m(X)/[M_r(X) \text{ g}] = n(X)/\text{mol} \quad (3)$$

We see immediately that when $n(X) = 1 \text{ mol}$, then $N(X) = g/\text{Da}$ (the Avogadro number), independent of the substance involved, and $m(X) = M_r(X) \text{ g}$ —“a mass that, when expressed in grams, has a numerical value exactly equal to the relative entity mass of the substance.” These are the physically based equations that should be used in stoichiometric calculations. Being homogeneous linear equations, they are easily understood by beginning science students—in stark contrast to traditional methods involving rote learning of the use of mysterious (and erroneously named) “conversion factors” that do not appear to be based on any discernable physical principles.