

On Feb 18, 2014, at 11:00 AM, Ian Mills wrote:

Dear Brian Leonard (Benny Leonard),

I have now read your document, and I shall attempt to provide you with my thoughts.

I fully agree with you that “chemical amount” would be a better name for the quantity than “amount of substance”. I have been trying to push that name for more than 20 years, but it has never really caught on. Since it is not used by anyone but a select few, I have continued to use the name amount of substance (or AoS for brevity) in what follows.

I appreciate that you have thought deeply about this subject. The difficulty is that the result of your thoughts (with some of which I have some sympathy) is that you have set up a new system of quantities and units that you regard as preferable to that used in the SI, but which is different from that used in the SI in a number of important ways. This has then led you into introducing new names for a number of the quantities and units involved, or sometimes introducing different meanings for some of the names currently used in the SI. That makes your document difficult to read, for me, and probably for most ordinary folk (such as chemists in general). I personally found I had to work hard to read your document. I am not sure that many of your intended readers will seriously attempt to go through your document.

For example, you wish to introduce “entity” as the base unit for AoS, and somehow treat the mole as a sort of derived unit equal to  $6.022\dots\times 10^{23}$  entities. You wish to have only one quantity that embraces N and n as being dimensionally the same. That is not what is done in the SI. Much follows from that. (See the appendix to this message that I have added below.) Introducing the ent is, perhaps, possible, but it has its problems; sometimes you need it and sometimes it leads to confusion. You have used lots of new names and symbols that I have to work on, such as “amount-specific-mass” (does that mean the quantity AoS/mass ?). Because your language is not familiar to me it is hard work.

In the SI there are many well accepted names and symbols, and I believe one

has to fall in with most of that in order to carry the community along with you. I have tried to summarise some of that language on the attached file. The IUPAC Green Book is a more general reference for the accepted language of science in the field of physical chemistry and chemical physics; the file I attach here is a small summary from the Green Book. The ISO/TC12 publications, particularly the ISO 31 series on Quantities and Units, now transformed into the ISO/IEC 80000 series, is also a general reference (which I find more difficult to use). I hope that you may find my attached file useful. The language summarized in my file is also widely presented in many text books of physical chemistry (Atkins' books for example). I think you will have to recognise and use the currently accepted language, at least to a large extent, if you are to make progress with your new ideas. Otherwise I fear that you will not get off the ground. I have been in this field for more than 20 years, and I am familiar with the difficulty of persuading the world to adopt radically new ideas.

You may also find our provisional draft for the next edition of the SI Brochure, which is available on the BIPM website, useful; I also attach a copy of that for your convenience. It is provisional, please respect that. The CCU is working on what to say about dimensionless quantities in the SI, but that is yet to come!

I am going to stop here for now. I send you good wishes. Ian 18feb2014

Appendix:

I think it is important to always clearly distinguish quantities (e.g. length, mass, time,...) from units (metre, kilogram, second,...). Quantity equations should remain unchanged regardless of what units you choose to use. One of the difficulties in introducing units for dimensionless quantities like the entity (or molecule) is that they somehow provide information on the quantity at the same time as acting as a unit.

There can be only one coherent unit for each quantity. In the SI the quantities AoS,  $n$ , and number of entities,  $N$ , are dimensionally different. Hence the different symbols. They are related by the Avogadro constant, which has the dimension of reciprocal mole in the SI (ent/mol if you wish). If you make  $n$  and  $N$  dimensionally the same there should be only one symbol. Similarly  $R$  and  $k$  become the same quantity and should have only one symbol. Similarly for  $F$  and  $e$ . These consequences and their ramifications will totally transform the language of science that is at present used by chemists all over the world.

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<i>Recommended notation for quantities</i>	<i>unit</i>	<i>coherent SI</i>
$m_s$	mass of sample s	kg
$n_s$	amount of substance (AoS), or chemical amount, of sample s	mol
$N_s$ (or ent)	number of entities of sample s  (for both $n_s$ and $N_s$ the entity must be defined; it could be one atom, or one molecule, or $\frac{1}{2}\text{O}_2$ , or $(1/5)\text{KMnO}_4$ , see Green Book 3 <sup>rd</sup> edn, 2007, p.53-54; 2 <sup>nd</sup> edn, 1993, p.46)	1 (d'less)
$N_A$ (or $L$ ) ent/mol)	Avogadro constant	$\text{mol}^{-1}$ (or
$p$	pressure	$\text{N/m}^2 = \text{Pa}$
$V$	volume	$\text{m}^3$
$R$	molar gas constant	$\text{J mol}^{-1} \text{K}^{-1}$
$T$	thermodynamic temperature	K
$k$ (or $k_B$ ) ent <sup>-1</sup> K <sup>-1</sup> )	Boltzmann constant	J/K (or J
$F$	Faraday constant	C/mol
$e$	elementary charge	C (or C/ent)
$M, M(X)$	molar mass (of molecule or entity X)	kg/mol
$M_u$	molar mass constant = $M(^{12}\text{C}) / 12 = N_A \times m_u$ (= 1 g/mol exactly in the current SI)	kg/mol
$m_u = 1 \text{ u} = 1 \text{ Da}$ kg/ent)	unified atomic mass constant = $m(^{12}\text{C}) / 12$  (dalton, symbol Da, is an alternative name for the unit u)	kg (or
$m(X)$ kg/ent)	mass of entity X	kg (or

$A_r(X)$ (or ent ?)	atomic or molecular weight of entity X  (relative atomic or molecular mass, scaled to $A_r(^{12}\text{C}) = 12$ )	1 (d'less)
$c$ , or $c(X)$	molar concentration of X in a solution, or the amount concentration of X, or the molarity of X (also often simply called the concentration of X by chemists)	$\text{mol/m}^3$
$\rho$ , or $\rho(X)$	mass concentration of X in a solution (also used for the mass density of a sample)	$\text{kg/m}^3$

Note that the unit quoted in the final column is the coherent SI unit, which is often not the commonly used unit (coherent units involve no multiple or sub-multiple prefixes, with the exception of the kg which is the coherent unit of mass). Thus the commonly used unit of molar mass is g/mol rather than kg/mol, and the commonly used unit of amount concentration is  $\text{mol/dm}^3 = \text{mol/L}$  rather than  $\text{mol/m}^3$ , etc. The commonly used unit of atomic mass is the u (= Da), which is not an SI unit. The name dalton is used mainly by large molecule chemists; unified atomic mass unit is the name used mainly by physicists. Note that the same symbol  $A_r(X)$  is used for the relative mass of both atoms and molecules.

If you were to introduce the unit entity, symbol ent, I have added in red some of the places where it would appear. It is the same as the unit molecule, symbol mol, in my original paper. Entity is perhaps a better name since it is more general, but it will be unfamiliar to most people. In the SI this unit is equal to one, 1.

The quantity amount of substance (AoS for brevity),  $n$ , and hence the Avogadro constant,  $N_A$ , may also be defined by the equations in which they occur with other quantities. This is illustrated in the equations below. These are examples of the equations of physics.

<i>Quantity equation</i>		<i>coherent SI units of the eqns</i>	
$n = N / N_A$	(AoS) = (No of entities) / (Avogadro const)	(mol) = (1) / (mol <sup>-1</sup> )	(1)
$n_s(X) = m_s / M(X)$	(AoS) = (mass of sample s) / (molar mass of X)	(mol) = (kg) / (kg/mol)	(2)
$pV = n RT$ $= N kT$	(ideal gas equation)	(N/m <sup>2</sup> ) (m <sup>3</sup> ) = (mol)(J mol <sup>-1</sup> K <sup>-1</sup> )(K) = (1) (J K <sup>-1</sup> ) (K)	(3a) (3b)
$R = N_A k$	(molar gas const) = ( $N_A$ ) × (Boltz const)	(J mol <sup>-1</sup> K <sup>-1</sup> ) = (mol <sup>-1</sup> )(J K <sup>-1</sup> )	(4)
$F = N_A e$	(Faraday const) = ( $N_A$ ) × (elementary charge)	(C/mol) = (mol <sup>-1</sup> ) (C)	(5)
$M(X) = N_A m(X)$	(molar mass) = ( $N_A$ ) × (mass of X)	(kg/mol) = (mol <sup>-1</sup> ) (kg)	(6)
$M(X) = A_r(X) M_u$	(molar mass) = (molecular wt) × (molar mass const)	(kg /mol) = (1) (kg/mol)	(7)
$A_r(X) = m(X) / u$	relative atomic or molecular weight of X = $m(X) / [m(^{12}\text{C})/12]$	(1) = (kg) / (kg)	(8)
$c_s(X) = n_s(X) / V$	(AoS concn) = (AoS) / (volume)	(mol/m <sup>3</sup> ) = (mol) / (m <sup>3</sup> )	(9)
$\rho_s = m_s / V$	(mass concn) = (mass of solute) / (volume)	(g/m <sup>3</sup> ) = (g) / (m <sup>3</sup> )	(10)
$c(X) = \rho_s / M(X)$	(AoS concn) = (mass concn) / (molar mass)	(mol/m <sup>3</sup> ) = (g/m <sup>3</sup> ) / (g/mol)	(11)

Note that it is generally agreed that “amount of substance” is not a good name, but although many other names have been suggested none has become generally accepted (see the discussion on p.4 of the IUPAC Green Book, 3<sup>rd</sup> edn (2007)). My own choice would be “chemical amount”, which can be conveniently abbreviated to the single word “amount” in examples like “amount concentration”. Chemists all use the unit mole, but most chemists never bother to consider the name of the quantity of which the mole is the SI unit. If pushed they would probably say “number of moles” which should be strongly discouraged.

I have not attempted to re-write the equations in the second column with the introduction of the unit entity, symbol ent, which would be equal to one in the SI. A few examples would be as below.

(4): the SI unit of  $N_A k$  would be (ent/mol)(J K<sup>-1</sup> ent<sup>-1</sup>)

(5): the SI unit of  $N_A e$  would be (ent/mol)(C/ent)

(6): the unit of  $N_A m(X)$  would be (ent/mol)(kg/ent)