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An Analytical Approach to Comprehending Fundamental Atomic Mass-Related Definitions

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Abstract This paper offers a clear framework for understanding basic atomic concepts.Throughout the manuscript, mass expressions are described as scalar quantitiesthatare characterized by a symbol, a numerical value, and a unit of measurement.It defines the role of the IUPAC ratio A_r ,explains the meaning of absolute and relative atomic mass, and determines the origin and relationship among molar mass, Avogadro's number, and the amount of substance. The approach moves from isolated isotopes to poly-isotopic elements, and from absolute atomic mass to relative atomic mass when applicable.The atomic mass ratio, A_r , plays an important role in this work. Absolute atomic mass, a magnitude expressed in kilograms, differs from relative atomic mass, denoted by the numerical value A_r with the unified atomic mass unit "u" . The relationship between the ratio A_r and the periodic table of elements is highlighted, emphasizing factors, besides the controversy between atomic mass and atomic weight, that may confuse users of the table.The concept of any mass quantity, "AMQ" ,is introduced to clarify the meaning of the atomic mass-weighted average. Furthermore, the idea "AMQ" in conjunction with the ratio A_r is used to demonstrate the origin and relationship among molar mass, Avogadro's number, and the amount of substance.

Keywords: *scalar quantity, IUPAC ratio A_r, absolute and relative atomic mass, molar mass, Avogadro´s Number, amount of substance*

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1. Introduction

Some concepts remain difficult for students and even instructors to grasp. Two instances include the interpretation of atomic mass (also referred to as atomic weight) as a dimensionless value on the periodic table, as well as the justification for obtaining the molar mass of an element.

Efforts to clearly explain the mole, Avogadro's number, the molar mass, and the amount of substance, along with ongoing discussions about potential future changes to the definition of the amount of substance "n," have been extensively documented in numerous publications [1,2,3,4,5,6].

The International Union of Pure and Applied Chemistry (IUPAC) has designated the symbol A_r to denote relative atomic mass (atomic weight), textually defined as "the ratio of the average mass of the atom to the unified atomic mass unit" [7,8]. However, the ratio A_r is not commonly mentioned in chemistry textbooks and publications, resulting in atomic mass-related explanations that are usually qualitative or based only on numerical examples rather than broader scope symbolic expressions [9].

The objective of this publication is to provide a comprehensive and systematic theoretical framework that elucidates and interconnects all definitions of atomic mass concepts.

2. The Atomic Mass as a ScalarQuantity

The atomic mass is a scalar quantity, and any scalar quantity is made up of a symbol, a magnitude or numerical value (nv), and a unit of measurement. Figure 1 resumes the way of representing a scalar quantity.

$$\boxed{Symbol = (nv)[unit]}$$

Figure 1. Composition of a scalar quantity

According to the IUPAC publication [8], the atomic mass symbol for an isotope with a mass number "i" of element (E) is $m_a\left({}^{i}E\right)$, where (E) is the symbol of the element. In this paper, and following IUPAC nomenclature [7], the symbol "i" changes to "A." Therefore, the "absolute" atomic mass of an isotope is a scalar quantity with the kilogram as a unit, represented as:

$$m_a\left({}^{A}E\right) = (nv)_{m_a\left({}^{A}E\right)}[kg] \tag{1}$$

The unified atomic mass unit "u" (also known as the

Dalton "D_a") [7], defined and accepted by agreement between chemists and physicists in 1961 [1], is also a scalar quantity given by:

$$u = {m_a\left({}^{12}C\right)}\Big/{12} = {(nv)_{m_a\left({}^{12}C\right)}[kg]}\Big/{12} \quad (2)$$

The ratio of $m_a\left({}^{A}E\right)$ to "u" is known as the relative atomic mass $A_r\left({}^{A}E\right)$ [7]. In other words,

$$A_r\left({}^{A}E\right) = {(nv)_{m_a\left({}^{A}E\right)}}\Big/{\left({(nv)_{m_a\left({}^{12}C\right)}}\Big/{12}\right)} \quad (3)$$

The quantity $(nv)_{m_a\left({}^{A}E\right)}$ is unknown, but the ratio $A_r\left({}^{A}E\right)$ is available through the mass spectrometer. Mass spectrometers do not provide absolute atomic masses; they only give isotopic $A_r\left({}^{A}E\right)$ valuesas well as the percentage fraction of the natural isotopic abundance. Applying equation (3) to $\left({}^{12}C\right)$ gives $A_r\left({}^{12}C\right) = 12$. Samples of $\left({}^{12}C\right)$ are used to calibrate mass spectrometers to obtain $A_r\left({}^{A}E\right)$ values of other elements with $A_r\left({}^{12}C\right)$ as a reference.

As demonstrated subsequently, "u" is derived from Avogadro's number [10,11]. As a result, since $A_r\left({}^{A}E\right)$ and "u" are known, $m_a\left({}^{A}E\right)$ can also be expressed as a "relative" atomic mass, as shown below.

$$m_a\left({}^{A}E\right) = A_r\left({}^{A}E\right)u \quad (4)$$

Expression (4) is a scalar quantity with $A_r\left({}^{A}E\right)$ as the numerical value.

Table 1 shows the isotopic composition of element chlorine [12].

Table 1. Chlorine Isotopic Composition

Isotope	$x\left({}^{A}Cl\right)$	$A_r\left({}^{A}Cl\right)$
$\left({}^{35}Cl\right)$	0.7576	34.9688
$\left({}^{37}Cl\right)$	0.2424	36.9659

The following is an example of obtaining absolute atomic mass through the atomic mass unit "u". Let us apply equation (4) to isotope $\left({}^{35}Cl\right)$.

$$m_a\left({}^{35}Cl\right) = A_r\left({}^{35}Cl\right)u =$$

$$34.9688 \cdot \left(1.6605\text{x}10^{-27}\,kg\right) = 5.8066x10^{-26}\,kg$$

Unlike the extremely small numerical value of the "absolute" atomic mass, the magnitude of "u" allows the ratio $A_r\left({}^{A}E\right)$ to become a whole number with up to three digits and a decimal portion with a variable number of digits, which is easier to handle than the numerical value of the "absolute" atomic mass.It is important to emphasize that expression (4) is the complete version of the relative atomic mass, whereas the ratio $A_r\left({}^{A}E\right)$ is only the numerical value of that quantity. Despite that, IUPAC defines this ratio as the full representation of relative atomic mass [7].

The following text is an exact transcription of a passage found on page 267 of an IUPAC publication [8]:

"Thus, the atomic mass of 12C is 12 Da, and the atomic weight of 12C is 12 exactly. All other atomic weight values are ratios to the 12C standard value and thus are dimensionless numbers."

The revised text below is an example of how the ideas discussed in this section can be applied to enhance the original (Modifications are highlighted).

Thus, the relative atomic mass of $\left({}^{12}C\right)$ is 12 Da, and the numerical value of the relative atomicmass of $\left({}^{12}C\right)$ is 12 exactly. This number and all other relative atomic mass numerical values are ratios to the unified atomic mass unit and thus are dimensionless numbers.

3. The Ratio A_r and the Periodic Table of the Elements

Up to this point, only isolated isotopes were considered.For elements of more than one natural isotope, the atomic mass is a weighted average [13] represented by $m_a(E)$.

This section introduces the concept of anymass quantity "AMQ" to help understand the origin of the atomic mass-weighted average.For a sample with any number "N" of atoms of an element (E) with "j" natural isotopes,any mass quantity is given by,

$$AMQ(E) = \sum_{i=1}^{j}\left[x\left({}^{A_i}E\right)N \cdot m_a\left({}^{A_i}E\right)\right] \quad (5)$$

Where $x\left({}^{A_i}E\right)N$ is the percentage fraction of the natural isotopic abundance, this factor equals one for elements with only one natural isotope. Dividing by "N" on both sides of equation (5), it is obtained the atomic mass-weighted average,

$$AMQ(E)\Big/N = \sum_{i=1}^{j}\left[x\left({}^{A_i}E\right) \cdot m_a\left({}^{A_i}E\right)\right] \quad (6)$$

Therefore,

$$m_a(E) = \sum_{i=1}^{j}\left[x\left({}^{A_i}E\right) \cdot m_a\left({}^{A_i}E\right)\right] \quad (7)$$

In this way, a single theoretical quantity $m_a(E)$ is equivalent to the atomic mass of natural isotopes of element (E), and the element can be treated as if it only has one isotope. Dividing by "u" on both sides of equation (7), the result is the atomic mass-weighted average in terms of the numerical value of the relative atomic masses,

$$A_r(E) = \sum_{i=1}^{j}\left[x\left({}^{A_i}E\right)\cdot A_r\left({}^{A_i}E\right)\right] \quad (8)$$

Be careful not to confuse A_r with the atomic mass number A_i.

The following example shows how to compute the value $A_r(Cl)$. From Table 1 and applying equation (8):

$$A_r(Cl) = x\left({}^{35}Cl\right)\cdot A_r\left({}^{35}Cl\right) + x\left({}^{37}Cl\right)\cdot A_r\left({}^{37}Cl\right)$$
$$A_r(Cl) = 0.7576\cdot 34.9688 + 0.2424\cdot 36.9659$$
$$A_r(Cl) = 26.4924 + 8.9605$$
$$A_r(Cl) = 35.4529$$

Hence, the percentage contribution of each isotope in creating $A_r(Cl)$ is: 74.72% $\left({}^{35}Cl\right)$ and 25.20% $\left({}^{37}Cl\right)$. Most cells in the periodic table of elements display a decimal number named atomic mass or atomic weight. Regardless of the name, this quantity is just the ratio $A_r(E)$ as given in equation (8) and shown in Figure 2.

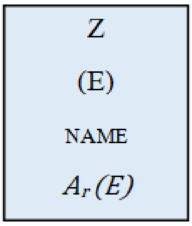

Figure 2. PeriodicTable cell (Z is the atomic number)

The remaining cells display whole numbers in parentheses, corresponding to the mass number of the most stable isotope among the unstable isotopes of radioactive elements [13].

Like isolated isotopes, the formula for the relative atomic mass of poly-isotopic elements is,

$$m_a(E) = A_r(E)u \quad (9)$$

Therefore, and as mentioned before, referring to the ratio $A_r(E)$ as the relative atomic mass or, even worse, atomic weight is confusing. Due to a lack of units, this ratio is only part of a scalar quantity, but not the whole scalar quantity as such. Even in the IUPAC Periodic Table of the Isotopes [8], which is a very complete source of information, neither the ratio $A_r(E)$ nor the unified atomic mass "u" are mentioned or related to the atomic weight (in this table, the term atomic weight is used instead ofatomic mass).

All the factors above can lead to confusion about the meaning of atomic mass or atomic weight in the periodic table. The following is a summary of them:

- A number without units is called atomic mass or atomic weight. Most periodic tables omit the unit "u".
- Given that the terms weight and mass are used indistinctly, it could seem that both concepts are equivalent at the atomic level.
- The ratio $A_r(E)$ and the word "atomic weight" are incompatible. This number is the numerical value of the "relative" atomic mass.

4. The Origin of Molar Mass, the Avogadro´s Number, and the Amount of Substance

The idea of "any mass quantity" "AMQ" already mentioned, togetherwith the ratio A_r is used to demonstrate through equations the origin as well as the relationship among the molar mass $M(E)$, the Avogadro´s number N_A, and the amount of substance "n" [14]. This approach also applies to molecules and ionic compounds.

Any mass quantity of any element (E) can be expressed as:

$$AMQ(E) = N\cdot m_a(E) = N\cdot A_r(E)\cdot u \quad (10)$$

Where N is the number of atoms.

Substituting "u" from equation (2) it is obtained,

$$AMQ(E) = N\cdot A_r(E)\left\{ (nv)_{m_a\left({}^{12}C\right)}[kg] \Big/ 12 \right\} \quad (11)$$

If the expression (11) is given in terms of grams, it will be equal to:

$$AMQ(E) = A_r(E)[g]\left[10^3 N\left\{ (nv)_{m_a\left({}^{12}C\right)} \Big/ 12 \right\}\right] \quad (12)$$

Let denote the numerical factor within square brackets as "n". Hence,

$$n = 10^3 N\left\{ (nv)_{m_a\left({}^{12}C\right)} \Big/ 12 \right\} \quad (13)$$

Where "n" could be any positive number.

Combining expressions (12) and (13) yields:

$$AMQ(E) = n\cdot A_r(E)[g] \quad (14)$$

and if $n = 1$ the expression (14) becomes the molar mass $M(E)$, formerly known as "gram atomic weight" [13]. Therefore, expression (14) can be rewritten as

$$M(E) = A_r(E)[g] \quad (15)$$

Expression (15) shows that the molar mass is a scalar quantity with the ratio $A_r(E)$ as the numerical value. The relative atomic mass (9) also has $A_r(E)$ as the numerical value. For that reason, there is a wrong tendency to think that the molar mass comes from an arbitrary change of units, "u" for g in expression (9) [2,3,4,5,6,7,8,9], without considering the numerical factor "n".

Also, if "n" equals 1, the number of atoms N in equation (13) is equal to Avogadro's number N_A which, once cleared, gives

$$N_A = 10^{-3} \Big/ \left\{ (nv)_{m_a(^{12}C)} \Big/ 12 \right\} \qquad (16)$$

Since "n" is always equal to one for the molar mass, it means that the molar mass of any element always has N_A atoms.

Regarding expression (16) and contrary to what might be assumed, N_A is derived from experimental work, and relation (16) is used only to compute the numerical value of "u" [4,10].

Figure 3 summarizes the relationship between different mass amounts and the corresponding number of atoms for element *(E)*.

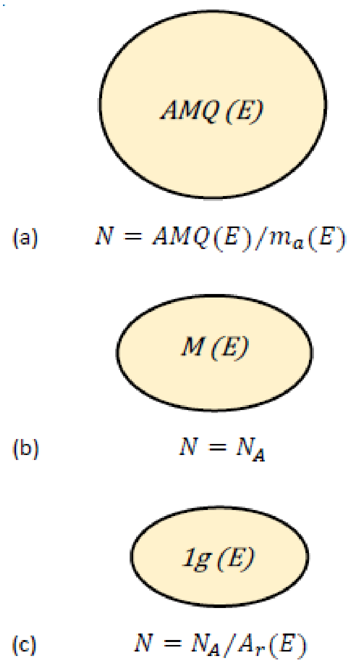

Figure 3. The number of atoms for different masses of an element *(E)*

From equations (13) and (16), it is found that "n" is just the ratio of N to N_A, which shows that "n" is precisely the amount of substance; therefore,

$$n = N \big/ N_A \qquad (17)$$

Where $N_A = 1mol = 6.022x10^{23}$

From the ratio (17), it is deduced that "n" represents the number of moles that fit in N, which suggests that "amount of moles" would be a better name for "n" than "amount of substance"when the entities are atoms.As an alternative, equation (17) can be rearranged into a scalar quantity as shown below

$$N = n[mol] \qquad (18)$$

where "n" is the numerical value and $[mol]$ the measurement unit.

5. Scalar Quantities and Measurement Units

Table 2 shows the scalar quantities covered in this article, emphasizing the units of measurement. Except for the unified atomic mass unit "u", all other units are SI base units. However, "u" is accepted for use with SI units [14].

Table 2. Scalar quantities

	Absolute atomic mass	Unified atomic mass unit	Relative atomic mass	Molar mass	Number of atoms
Expression	$m_a(E) = (nv)_{m_a(E)}[kg]$	$u = (nv)_{m_a(^{12}C)}[kg]/12$	$m_a(E) = A_r(E)[u]$	$M(E) = A_r(E)[g]$	$N = n[mol]$
Measure unit name	kilogram	kilogram	Atomic mass unit	gram	mole
Measure unit symbol	kg	kg	u	g	mol

6. Conclusions

Remembering that mass is a scalar quantity is the first step in understanding atomic mass-related basic concepts.

The ratio A_r is not popular as a symbol for educational purposes. It is uncommon to find it in chemistry textbooks, even though there is no other symbol equivalent to A_r. The use of the IUPAC ratio A_r should be expanded throughout the field of science education to standardize nomenclature and enhance the teaching and learning processes.

Recognizing the decimal number in some cells of the periodic table of the elements as the ratio A_r reveals that it is wrong to refer to this number as the relative atomic mass or atomic weight. Without the unit *"u* ? this number is not a complete scalar quantity. To be accurate, it is only the numerical value of the relative atomic mass and not the whole scalar quantity as erroneously stated by IUPAC [7]. Those mentioned above,besides the controversy between mass and weight,are a main source of confusion among students and even teachers.

Introducing the idea of any mass quantity, "*AMQ*" besides being useful in defining the weighted average atomic mass, has been fundamental in providing a sound demonstration that explains the origin and relationship among the molar mass, Avogadro´s number, and the amount of substance. It eliminates the need to use or seek out qualitative definitions, official or not, that could help describe these concepts.

Substituting "*u*" for grams in the expression for relative atomic mass to obtain molarmass is only a rule of thumb that disguises the true origin of molar mass.Choosing grams as a unit for molar mass is a matter of convenience. If given in kilograms, the only change is that Avogadro's number would increase by a factor of one thousand.

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