LETTER TO THE EDITOR

Molar mass and related quantities in the New SI

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Abstract
This letter addresses the calculation of molar mass and related quantities in the updated version of the SI (most often called the 'New SI' but sometimes the 'Quantum SI') currently under discussion by the International Committee for Weights and Measures and its Consultative Committee for Units and which could be adopted by the next General Conference on Weights and Measures in 2011.

1. Introduction

There is a reasonable likelihood that the next General Conference on Weights and Measures, the 24th and which is to convene in 2011, will adopt new definitions of the kilogram, ampere, kelvin and mole based on fixed values of the Planck constant h, elementary charge e, Boltzmann constant k and Avogadro constant N_A, respectively, just as the current definition of the metre is based on a fixed value of the speed of light in vacuum c [1–3]. (In this letter the current International System of Units, or SI, is simply called 'SI' while the International System of Units with the new definitions is called 'New SI.')

Whereas in the SI the definitions of the kilogram, ampere, kelvin and mole fix the values of the mass of the international prototype of the kilogram $m(\mathcal{K})$, the magnetic constant μ_0, the triple point of water T_{TPW} and the molar mass of the carbon-12 atom $M(^{12}C)$ to be exactly $1\,kg$, $4\pi \times 10^{-7}\,N\,A^{-2}$, $273.16\,K$ and $12\,g\,mol^{-1}$, respectively, in the New SI these quantities no longer have exact values but must be determined experimentally.

One of the consequences of $M(^{12}C)$ no longer being exactly $12\,g\,mol^{-1}$ is that the molar mass of an entity X, $M(X)$, can no longer be calculated from the expression $M(X) = A_r(X)\,g\,mol^{-1}$, but must be calculated from a modified form of this expression [2]. (As usual and as defined in (14), the quantity $A_r(X)$, formerly called the 'atomic weight' of X, is the relative atomic mass of X.) The purpose of this letter is to present a straightforward way of calculating $M(X)$ and related quantities that avoids the use of the molar mass factor $(1 + \kappa)$ introduced in [2] while at the same time retaining the current definitions of the relevant quantities and constants, thereby simplifying molar mass calculations in particular and the New SI in general[2].

2. Summary of results

2.1. Definitions

For easy reference, the relevant constants, quantities and relations among them are summarized in this section. Note that all the equations that appear in (1)–(23) apply to both the SI and the New SI, and that derivations of the most important of these equations are given in the appendix.

c	speed of light in vacuum (exactly known in the SI and the New SI)	(1)
h	Planck constant (exactly known in the New SI)	(2)
e	elementary charge (exactly known in the New SI)	(3)
m_e	electron mass	(4)
α	fine-structure constant: $\alpha = \mu_0 c e^2/2h$	(5)
R_∞	Rydberg constant: $R_\infty = \alpha^2 m_e c/2h$	(6)

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N_A Avogadro constant (number of specified entities X per mole and exactly known in the New SI)   (7)

$m(X)$ mass of entity X (8)

$m(^{12}C)$ mass of the carbon-12 atom   (9)

$M(X)$ molar mass of entity X (mass per amount of substance of X): $M(X) = m(X)N_A$ (10)

$M(^{12}C)$ molar mass of the carbon-12 atom: $M(^{12}C) = m(^{12}C)N_A$ (in the SI the definition of the mole fixes the value of $M(^{12}C)$ to be 12 g mol^{-1} exactly, but not in the New SI)   (11)

m_u atomic mass constant: $m_u = m(^{12}C)/12$ (12)

u   unified atomic mass unit (also called the dalton, symbol Da): $1\,u = 1\,Da = m_u$ (13)

$A_r(X)$ relative atomic mass of entity X: $A_r(X) = m(X)/m_u$ (14)

$A_r(^{12}C)$ relative atomic mass of the carbon-12 atom: $A_r(^{12}C) = m(^{12}C)/m_u = 12$ exactly in the SI and the New SI   (15)

$A_r(e)$ relative atomic mass of the electron: $A_r(e) = m_e/m_u$ (16)

M_u molar mass constant: $M_u = M(^{12}C)/12$ (since $M(^{12}C) = 12$ g mol^{-1} exactly in the SI, $M_u = 1$ g mol^{-1} exactly in the SI, but not in the New SI)   (17)

$n_S(X)$ amount of substance of X for a sample S of entities X: $n_S(X) = N_S(X)/N_A = m_S(X)/M(X)$, where $N_S(X)$ is the number of entities X in the sample and $m_S(X)$ is the mass of the sample (again, these relations hold in both the SI and the New SI)   (18)

2.2. Expressions for calculating molar mass and related quantities

The relevant expression for calculating the molar mass $M(X)$ of an entity X is

$$M(X) = A_r(X)\frac{M(^{12}C)}{12} = A_r(X)M_u \qquad (19)$$

with

$$\frac{M(^{12}C)}{12} = M_u = \frac{2R_\infty N_A h}{\alpha^2 c A_r(e)}. \qquad (20)$$

The expressions for the related quantities $m(X)$, $m(^{12}C)$ and $1\,u = 1\,Da = m_u$ are

$$m(X) = \frac{A_r(X)}{N_A}\frac{M(^{12}C)}{12} = \frac{A_r(X)M_u}{N_A}, \qquad (21)$$

$$m(^{12}C) = \frac{12}{N_A}\frac{M(^{12}C)}{12} = \frac{12 M_u}{N_A}, \qquad (22)$$

$$1\,u = 1\,Da = m_u = \frac{1}{N_A}\frac{M(^{12}C)}{12} = \frac{M_u}{N_A}. \qquad (23)$$

Although (19)–(23) hold for both the SI and the New SI, the SI definition of the mole is such that $M(^{12}C)/12 = M_u = 1$ g mol^{-1} exactly, as already indicated. Consequently, in the

SI the combination of constants on the right-hand side of (20) has this value.

2.3. Evaluation of expressions and application

If the New SI were to be implemented today based on the results of the most recent (2006) Committee on Data for Science and Technology (CODATA) least-squares adjustment, one would have for the constants of interest [4]

$c = 299\,792\,458$ m s^{-1} (exact),

$h = 6.626\,068\,961 \times 10^{-34}$ J s   (exact),

$N_A = 6.022\,141\,794 \times 10^{23}$ mol^{-1} (exact),

$R_\infty = 10\,973\,731.568\,527(73) \times 10^7$ m^{-1} $[6.6 \times 10^{-12}]$,

$A_r(e) = 5.485\,799\,0943(23) \times 10^{-4}$ $[4.2 \times 10^{-10}]$,

$\alpha = 1/137.035\,999\,679(94)$ $[6.8 \times 10^{-10}]$,

$$(24)$$

where one additional digit has been included in the values of h and N_A beyond those given in the 2006 CODATA compilation to reduce rounding errors in the calculations below.

To ensure that the consistency of the New SI with the SI is at an acceptable level, the fixed values of h and N_A chosen to redefine the kilogram and the mole must be such that the difference between the magnitudes (sizes) of the New SI kilogram and the SI kilogram and the difference between the magnitudes of the New SI mole and the SI mole have no practical consequences and may therefore be considered negligible. This means that in establishing the New SI, one is not free to choose arbitrary values for any of the constants in (24), in particular for h and N_A, but only values that result from a least-squares adjustment in which all quantities are expressed in their respective SI units, since such adjustments provide a set of self-consistent SI values of the constants that satisfy (20) [4].

The values of the constants in (24) together with (20), (22) and (23) lead to

$M(^{12}C)/12$

$$= M_u = 1.000\,000\,0000(14)\ \text{g mol}^{-1}\ [1.4 \times 10^{-9}] \qquad (25a)$$

$$= [1 + 0.0(1.4) \times 10^{-9}]\ \text{g mol}^{-1}\ [1.4 \times 10^{-9}],$$

$$m(^{12}C) = 1.992\,646\,5384(28) \times 10^{-26}\ \text{kg}\ [1.4 \times 10^{-9}], \qquad (25b)$$

$1\,u = 1\,Da$

$$= m_u = 1.660\,538\,7820(24) \times 10^{-27}\ \text{kg}\ [1.4 \times 10^{-9}], \qquad (25c)$$

where the covariances among R_∞, $A_r(e)$ and α are sufficiently small that they have a negligible effect on the uncertainty of $M(^{12}C)/12 = M_u$. Because the fixed values of h and N_A are the self-consistent recommended values resulting from the 2006 CODATA least-squares adjustment in which all quantities

are expressed in SI units, the magnitudes of the New SI kilogram and mole are highly consistent with the magnitudes of the SI kilogram and mole. It is therefore no surprise to see from (25a) that in the New SI, $M(^{12}C)/12 = M_u$ is equal to $1\,g\,mol^{-1}$ within its fractional uncertainty of 1.4×10^{-9}.

As an example of the calculation of the molar mass of a real substance, we consider silicon. Naturally occurring Si has three isotopes: ^{28}Si, ^{29}Si and ^{30}Si. In the most recent International Union of Pure and Applied Chemistry (IUPAC) compilation of the atomic weights of the elements dated 2005 [5], its relative atomic mass is given as $A_r(Si) = 28.0855(3)$. Thus the molar mass of naturally occurring silicon would be, from (19) and the above value of $M(^{12}C)/12 = M_u$,

$$M(Si) = 28.0855(3) \times 1.000\,000\,0000(14)\,g\,mol^{-1}$$

$$= 28.0855(3)\,g\,mol^{-1}.$$

Clearly, the numerical value and uncertainty of $M(^{12}C)/12 = M_u$ has no practical effect on the value of $M(Si)$ obtained from $A_r(Si)$. (Because atomic weight, or more correctly relative atomic mass, is defined according to (14), namely, $A_r(X) = m(X)/m_u$, it is a dimensionless quantity. Thus the periodic IUPAC compilations of the atomic weights of the elements do not depend directly on a particular set of units such as the SI or the New SI.)

Further, we may now answer a question such as 'What is the amount of substance of Si for a 100 g sample S of naturally occurring Si?' From (18) we have

$$n_S(Si) = N_S(Si)/N_A = m_S(Si)/M(Si)$$

$$= 100\,g/[28.0855(3)\,g\,mol^{-1}] = 3.56\,mol.$$

It is expected that the recommended values resulting from the 2010 CODATA least-squares adjustment will serve as the basis for the exact values of h, e, k and N_A chosen for the new definitions if, as anticipated, they are adopted by the 24th CGPM in 2011. However, it should be recognized that CODATA adjustments of the values of the constants subsequent to that of 2010, for example that of 2014, will undoubtedly lead to small changes in M_u, $m(^{12}C)$ and m_u, because the recommended values of R_∞, $A_r(e)$ and α on which they depend (see (20)–(23)) would likely change slightly from one adjustment to the next due to new data. Nevertheless, it is highly probable that any changes in M_u, $m(^{12}C)$ and m_u would be less than 2×10^{-9} in relative value, which would be so small that they would have no practical consequences of any sort. Of course, because they would be fixed by the new definitions of the kilogram and mole, the recommended values of h and N_A would not change and hence would not themselves lead to any change in M_u, $m(^{12}C)$ or m_u. This is analogous to the speed of light in vacuum: because the value of c is fixed by the definition of the metre, it does not change from one adjustment to the next.

2.4. The molar mass constant M_u

In the above discussion we have used the molar mass constant M_u, which we have defined to be equal to $M(^{12}C)/12$ exactly,

in both the SI and the New SI. The convenience of adopting this constant, with this name and symbol, is that it is for molar mass the analogue of the atomic mass constant m_u, which is defined to have the value $m(^{12}C)/12$. These two constants are related by the equation $M_u = m_u N_A$. It then enables us to write the molar mass of an atom (or molecule) X as in (19), $M(X) = A_r(X)M_u$, just as we write the mass of an entity X in u (sometimes incorrectly called atomic mass) in the form $m(X) = A_r(X)m_u$.

To reiterate, in the SI, $M_u = 1\,g\,mol^{-1}$ exactly, but in the New SI the value of M_u will no longer be exactly known. Although it will have this same value at the time of adoption of the New SI (see (25a)), the value will have an associated uncertainty, and, as already observed, the value may change slightly from the value $1\,g\,mol^{-1}$ due to future changes in the adjusted values of R_∞, $A_r(e)$ and α due to new data. However, the fractional change of M_u from the value $1\,g\,mol^{-1}$ is unlikely ever to be greater than a few parts in 10^9, and this is so much smaller than the uncertainty with which chemical measurements are likely to be made that for all practical purposes chemists may still treat M_u as being exactly equal to $1\,g\,mol^{-1}$.

The constant M_u with the name 'molar mass constant' has not been much used in the established literature. It can, of course, always be replaced by the expression $M(^{12}C)/12$, which is how it is defined—as one-twelfth of the molar mass of carbon-12. We recommend that this constant could be used with advantage more widely than it is at present, in teaching chemistry for example, to simplify the expression for calculating the molar mass of atoms and molecules.

Appendix. Derivation of expressions

From the quotient of (10) and (11) one has

$$M(X) = \frac{m(X)}{m(^{12}C)} M(^{12}C),$$

which, with the aid of (12) and (14), becomes (19):

$$M(X) = A_r(X) \frac{M(^{12}C)}{12}.$$

From (6) one has

$$m_e = \frac{2R_\infty h}{\alpha^2 c},$$

which may be written as

$$m(X) = \frac{2R_\infty h m(X)}{\alpha^2 c m_e},$$

or, with the aid of (14) and (16), as

$$m(X) = \frac{2R_\infty h A_r(X)}{\alpha^2 c A_r(e)}.$$

Based on (10), this last expression leads to

$$M(X) = \frac{2R_\infty N_A h A_r(X)}{\alpha^2 c A_r(e)}.$$

If the entity X is the carbon-12 atom, then, with the aid of (15), this becomes (20):

$$\frac{M(^{12}C)}{12} = \frac{2R_\infty N_A h}{\alpha^2 c A_r(e)}.$$

Further, we see that (21) follows from (10) and (19), (22) is the same as (11), and (23) follows from (11) and (12).

For completeness, we point out that the molar mass factor $(1+\kappa)$ first introduced in [4], and the molar mass of carbon-12, are related by $(1+\kappa) = M(^{12}C)/(12\,\text{g mol}^{-1})$. Thus, with the aid of this expression, (19)–(23) could be rewritten in terms of $(1+\kappa)$. We also see from this expression that in the New SI, the difference between $M(^{12}C)$ and $12\,\text{g mol}^{-1}$ carries the same information that is carried by the factor $(1+\kappa)$.

Acknowledgment

References

[1] BIPM 2007 *Comptes Rendus des Séances de la 23rd Conférence Générale des Poids et Mesures* (the relevant CGPM resolution, No 12, is available at http://www.bipm.org/utils/en/pdf/Resol23CGPM-EN.pdf) (to be published)

[2] Mills I M, Mohr P J, Quinn T J, Taylor B N and Williams E R 2006 *Metrologia* **43** 227–46

[3] BIPM 2006 *The International System of Units* 8th edn (Sèvres, France: Bureau International des Poids et Mesures) http://www.bipm.org

[4] Mohr P J, Taylor B N and Newell D B 2008 *Rev. Mod. Phys.* **80** 633–730
   Mohr P J, Taylor B N and Newell D B 2008 *J. Phys. Chem. Ref. Data* **37** 1187–284

[5] Wieser M E 2006 *Pure Appl. Chem.* **78** 2051–66