Calculating Molar Mass and Related Quantities in the New SI

Barry N. Taylor, NIST, 27 July 2007
(barry.taylor@nist.gov)

1. Introduction

At the 18th meeting of the CCU held 11-12 June 2007 at the BIPM, some participants expressed concern about the molar mass factor $(1 + \kappa)$ introduced in Ref. [1] in the calculation of molar mass and related quantities in the new SI. It is seen as a potential source of confusion in the new SI presented in Ref. [1].

Whereas in the current 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 $M(^{12}\mathrm{C})$, respectively, in the new SI these quantities are no longer exactly known but must be determined experimentally. In their place, the Planck constant h, elementary charge e, Boltzmann constant k, and Avogadro constant N_{A} have exactly defined values as a result of the new definitions of the kilogram, ampere, kelvin, and mole, respectively.

One of the consequences of these changes is that the molar mass of an entity X, $M(X)$, can no longer be calculated from the expression $M(X) = A_{\mathrm{r}}(X)$ g/mol, but must be calculated from a modified form of this expression [1]. [As usual and as defined below, $A_{\mathrm{r}}(X)$ is the relative atomic mass of X.] The purpose of this note is to present a way of calculating $M(X)$ and related quantities without formally introducing the factor $(1 + \kappa)$, 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. 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 the entries (1) to (22) below apply to both the current and new SI.

(1) c speed of light in vacuum (exactly known in the current and new SI)

(2) h Planck constant (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: $R_\infty = \alpha^2\, m_{\mathrm{e}}\, c/2h$

(6) 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) $m(^{12}\mathrm{C})$ mass of the carbon-12 atom

(9) $M(X)$ molar mass of entity X (mass per amount of substance of X): $M(X) = m(X)\, N_{\mathrm{A}}$

(10) $M(^{12}\mathrm{C})$ molar mass of the carbon-12 atom: $M(^{12}\mathrm{C}) = m(^{12}\mathrm{C})\, N_{\mathrm{A}}$ (in the current SI the definition of the mole fixes the value of $M(^{12}\mathrm{C})$ to be 12 g/mol exactly, but not in the new SI)

(11) m_{u} atomic mass constant: $m_{\mathrm{u}} = m(^{12}\mathrm{C})/12$

(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 current and 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 exactly in the current SI, $M_u = 1$ g/mol exactly in the current 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 current and the new SI)

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

$$(18) \quad M(X) = A_r(X)\frac{M(^{12}\mathrm{C})}{12} = A_r(X)M_u$$

with

$$(19) \quad \frac{M(^{12}\mathrm{C})}{12} = M_u = \frac{2R_\infty N_A h}{\alpha^2 c A_r(\mathrm{e})}.$$

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

$$(20) \quad m(X) = \frac{A_r(X)}{N_A}\frac{M(^{12}\mathrm{C})}{12} = \frac{A_r(X)M_u}{N_A}$$

$$(21) \quad m(^{12}\mathrm{C}) = \frac{12}{N_A}\frac{M(^{12}\mathrm{C})}{12} = \frac{12M_u}{N_A}$$

$$(22) \quad 1\ \mathrm{u} = 1\ \mathrm{Da} = m_u = \frac{1}{N_A}\frac{M(^{12}\mathrm{C})}{12} = \frac{M_u}{N_A}.$$

Although (18)-(22) hold for both the new and the current SI, the current definition of the mole is such that $M(^{12}C)/12 = M_u = 1$ g/mol exactly, as already indicated. Consequently, in the current SI the combination of constants on the right-hand-side of (19) has this value.

If the new SI were to be implemented today based on the 2006 CODATA recommended values of the constants, one would have [2]

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

$h = 6.626\,068\,960\,8 \times 10^{-34}$ J s (exact)

$N_A = 6.022\ 141\ 794\ 3 \times 10^{23}\ \text{mol}^{-1}$ (exact)

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

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

$\alpha = 1/137.035\ 999\ 679(94)$ $[6.6 \times 10^{-10}]$,

where two additional digits have been included in the values of h and N_A beyond those given in the 2006 CODATA compilation to minimize rounding errors. In this regard, it should be recognized that to avoid discontinuities in the magnitudes of the kilogram and mole in going from the current SI to the new SI, the values of h and N_A chosen to redefine the kilogram and mole must be such that the difference between the magnitudes of the new and current kilogram and the difference between the magnitudes of the new and current mole are negligible. As a consequence, in establishing the new SI, one is not free to choose arbitrary values for any of the above constants, in particular for h and N_A, but only values that result from a least-squares adjustment, since such adjustments provide a set of self-consistent values that satisfy (19).

The above values of the fundamental constants and (19), (21), and (22) lead to

$$M(^{12}\text{C})/12 = M_u = 1.000\ 000\ 0000(14)\ \text{g/mol}\ \ [1.4 \times 10^{-9}]$$
$$= [1 + 0.0(1.4) \times 10^{-9}]\ \text{g/mol}\ \ [1.4 \times 10^{-9}]$$

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

$$1\ \text{u} = 1\ \text{Da} = m_u = 1.660\ 538\ 7820(23) \times 10^{-27}\ \text{kg}\ \ [1.4 \times 10^{-9}].$$

Because the fixed values of h and N_A have been chosen so that the magnitudes of the new kilogram and mole are consistent with the magnitudes of the current kilogram and mole, it is no surprise that $M(^{12}\text{C})/12 = M_u$ is very nearly equal to 1 g/mol.

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 IUPAC compilation of the atomic weights of the elements dated 2005 [3], its relative atomic mass is given as $A_r(\text{Si}) = 28.0855(3)$. Thus the molar mass of naturally occurring silicon would be, from (18) and the above value of $M(^{12}\text{C})/12 = M_u$,

$$M(\text{Si}) = 28.0855(3) \times 1.000\ 000\ 0000(14)\ \text{g/mol} = 28.0855(3)\ \text{g/mol}.$$

Clearly, the numerical value and uncertainty of $M(^{12}\text{C})/12 = M_u$ has no effect on the value of $M(\text{Si})$ obtained from $A_r(\text{Si})$.

Further, we may now answer a question such as "What is the amount of substance of Si for a 100 g sample of naturally occurring Si?" From (17) we have

$$n_S(\text{Si}) = N_S(\text{Si})/N_A = m_S(\text{Si})/M(\text{Si}) = 100\ \text{g}/[28.0855(3)\ \text{g/mol}] = 3.56\ \text{mol}.$$

Finally, it should be recognized that the value $M(^{12}\text{C})/12 = M_u = [1 + 0.0(1.4) \times 10^{-9}]$ g/mol given above as obtained from (19) using the 2006 CODATA recommended values would likely change slightly from one CODATA least-squares adjustment to the next when carried out after the new definitions are adopted, because the recommended values of R_∞, α^2, and $A_r(\text{e})$ would likely change slightly from one adjustment to the next due to new data. Of course, because they are fixed by the definitions of the kilogram and mole, the recommended values of h and N_A would not change. This is analogous to the speed of light in vacuum: because the value of c is fixed by the definition of the meter, it does not change from one adjustment to the next.

2.3 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 current SI and in the new SI proposed in Ref. [1]. 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 (18), $M(X) = A_r(X) M_u$, just as we write the atomic mass in the form $m(X) = A_r(X) m_u$.

It is important to note that in the current SI, $M_u = 1$ g/mol exactly, but in the new SI the value of M_u will no longer be exactly known. Although it will initially have this same value, it will have an uncertainty, and as already observed it may change slightly from the value 1 g/mol due to future adjustments of the values of other constants. However the relative change of M_u from the value 1 g/mol 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 equal to 1 g/mol.

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 A: Derivation of expressions

From the quotient of (9) and (10) one has

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

which, with the aid of (13) and (14), becomes (18):

$$M(X) = A_\mathrm{r}(X) \frac{M(^{12}\mathrm{C})}{12}.$$

From (5) one has

$$m_\mathrm{e} = \frac{2R_\infty h}{\alpha^2 c},$$

which may be written as

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

or, with the aid of (13) and (15), as

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

Based on (9), this last expression leads to

$$M(X) = \frac{2R_\infty N_\mathrm{A} h A_\mathrm{r}(X)}{\alpha^2 c A_\mathrm{r}(\mathrm{e})} .$$

If the entity X is the carbon-12 atom, then, with the aid of (14), this becomes (19):

$$\frac{M(^{12}\mathrm{C})}{12} = \frac{2R_\infty N_\mathrm{A} h}{\alpha^2 c A_\mathrm{r}(\mathrm{e})} .$$

Further, we see that (20) follows from (9) and (18); (21) is the same as (10); and (22) follows from (10) and (11).

For completeness, we point out that the molar mass factor $(1 + \kappa)$ first introduced in Ref. [1], and the molar mass of carbon 12, are related by $(1 + \kappa) = M(^{12}\mathrm{C})/(12\ \mathrm{g/mol})$. Thus, with the aid of this expression, (18)-(22) could be rewritten in terms of $(1 + \kappa)$. We also see from this expression that in the new SI, the difference between $M(^{12}\mathrm{C})$ and 12 g/mol carries the same information that is carried by the factor $(1 + \kappa)$.

Acknowledgements

The author gratefully acknowledges the critically important input to this document provided by his colleagues I. M. Mills, P. J. Mohr, T. J. Quinn, and E. R. Williams.

References

[1] I. M. Mills, P. J. Mohr, T. J. Quinn, B. N. Taylor, and E. R. Williams, Metrologia **43,** 227 (2006).

[2] The 2006 CODATA set of recommended values of the constants is available at http://physics.nist.gov/constants. A detailed paper describing the 2006 CODATA adjustment of the values of the constants authored by P. J. Mohr, B. N. Taylor, and D. B. Newell is in preparation and is expected to be submitted by the end of 2007 for publication.

[3] M. E. Wieser, Pure Appl. Chem. **78**, 2051 (2006).