IOP PUBLISHING METROLOGIA

Metrologia **49** (2012) 487–491 doi:10.1088/0026-1394/49/4/487

Why the dalton should be redefined exactly in terms of the kilogram

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Received 5 January 2012, in final form 24 April 2012
Published 29 May 2012
Online at stacks.iop.org/Met/49/487

Abstract

With a redefined kilogram fixing the Planck constant, h, and a redefined mole fixing the Avogadro constant, N_A, as recently proposed, retaining the carbon-12-based dalton creates a fundamental incompatibility in the stoichiometric equations. To avoid this incompatibility, the dalton should be redefined, as well: exactly in terms of the fixed-h kilogram. Specifically, with the mole defined as mol $= N^*/N_A$, where N^* is an exact dimensionless constant, the dalton should be redefined as Da $= (1/1000N^*)$ kg, exactly, so that N_A/mol^{-1} remains exactly equal to the gram-to-dalton mass-unit ratio—as required by the fundamental compatibility condition relating the kilogram, mole and dalton. This would necessarily decouple the dalton from the carbon-12 reference mass, $m_a(^{12}\text{C})/12$, used for cataloguing nuclidic mass ratios to extremely high precision. Relative atomic masses, defined as $A_r(\text{X}) = m_a(\text{X})/\text{Da}$, would then have uncertainties dominated by that of $m_a(^{12}\text{C})/\text{kg}$; but since this would be of order 10^{-9} or less, the values of relative atomic masses, to the precision used in stoichiometry, would be totally unaffected. This is a much more straightforward and easily comprehended strategy than those using confusing inexact correction factors or the equivalent, as recommended in recent publications and implicitly endorsed by the CGPM.

1. Introduction

The following is in response to the call by the BIPM for comments on proposed redefinitions of SI base units recently endorsed, in principle, by the CGPM [1]. Since the kilogram, mole and dalton are intimately related, it is important to stress that the current carbon-12-based dalton, implicitly retained with the new definitions, is *not compatible* with the combination of the proposed redefined fixed-Planck-constant kilogram and fixed-Avogadro-constant mole [2]. This incompatibility necessitates the use of either an explicit inexact correction factor [3] or equivalent strategies involving implicit correction factors [4, 5]. In all cases, the resulting stoichiometric equations are difficult to comprehend and would be practically impossible to teach to beginning science students in an understandable fashion.

If the proposed fixed-h kilogram and fixed-N_A mole redefinitions were to be adopted, the dalton should be redefined, as well, in a compatible manner. With the mole defined as mol $= N^*/N_A$, where N^* is an exact dimensionless constant, the compatible dalton needs to be redefined exactly in terms of the fixed-Planck-constant kilogram as Da $= 1/(1000N^*)$ kg, exactly—thereby guaranteeing that the numerical value of N_A, when N_A is expressed in reciprocal moles, i.e. N_A/mol^{-1}, *remains* exactly equal to the gram-to-dalton mass-unit ratio. To the precision used in stoichiometry, there is then no change in any of the values of relative atomic masses with this redefinition of the dalton. Some minor notational changes will be needed in cataloguing (to high precision) directly measured and distinctly defined 'nuclidic mass ratios,' which will still be based on the carbon-12 reference mass, now decoupled from the exact dalton.

2. The substance-mass and amount-of-substance equations

2.1. The fundamental definition of the mole

For notational simplicity, consider an atomic substance consisting of an aggregate of a single isotope, represented by the symbol X. This can easily be generalized to account for molecules, formula units and other kinds of specified entities and combinations of different isotopes. The total substance mass is $m(\text{X})$; the atomic mass is $m_a(\text{X})$; the total number of entities, $N(\mathrm{X})$, is therefore equal to $m(\mathrm{X})/m_\mathrm{a}(\mathrm{X})$. If the relative atomic mass is $A_\mathrm{r}(\mathrm{X}) = m_\mathrm{a}(\mathrm{X})/\mathrm{Da}$, we can express the substance mass as

$$m(\mathrm{X}) = N(\mathrm{X}) m_\mathrm{a}(\mathrm{X}) = N(\mathrm{X}) A_\mathrm{r}(\mathrm{X})\,\mathrm{Da}. \qquad (1)$$

The right-hand side consists of an extremely large number, $N(\mathrm{X})$, multiplied by a number of O(1), $A_\mathrm{r}(\mathrm{X})$, and an extremely small atomic-scale mass unit, Da. In practice, we need to express the substance mass in terms of a macroscopic unit; conventionally, this is taken to be the gram, g. Multiplying and dividing the right-hand side by g gives

$$m(\mathrm{X}) = [N(\mathrm{X})/(\mathrm{g}/\mathrm{Da})] A_\mathrm{r}(\mathrm{X})\,\mathrm{g}. \qquad (2)$$

The term in square brackets is of O(1): $N(\mathrm{X})$ has been normalized by the characteristic dimensionless parameter g/Da, the gram-to-dalton mass-unit ratio—i.e. the atomic-to-macroscopic scale factor for mass.

By definition, the total amount of substance in a sample, $n(\mathrm{X})$, is related to the corresponding number of entities in the sample by

$$n(\mathrm{X}) = N(\mathrm{X})/N_\mathrm{A}, \qquad (3)$$

where N_A is the Avogadro constant, the only defined property of which is that it is indeed a constant (i.e. independent of X) with the dimension of reciprocal amount of substance. In order to relate amount of substance to the (easily measured) substance mass expressed in grams, we need to normalize $N(\mathrm{X})$ in equation (3) by *exactly the same factor* that appears in equation (2), giving

$$n(\mathrm{X}) = [N(\mathrm{X})/(\mathrm{g}/\mathrm{Da})](\mathrm{g}/\mathrm{Da})/N_\mathrm{A}. \qquad (4)$$

Since $N(\mathrm{X})/(\mathrm{g}/\mathrm{Da})$ is dimensionless and of O(1), the term $(\mathrm{g}/\mathrm{Da})/N_\mathrm{A}$—a macroscopic constant with the dimension of amount of substance—forms a natural macroscopic unit for this quantity. This is the source of the fundamental definition of the mole:

$$\mathrm{mol} = (\mathrm{g}/\mathrm{Da})/N_\mathrm{A}, \text{ exactly}. \qquad (5)$$

Note that this implies: $N_\mathrm{A}\mathrm{Da} = \mathrm{g\,mol}^{-1}$, exactly, and in particular that $N_\mathrm{A} = (\mathrm{g}/\mathrm{Da})\,\mathrm{mol}^{-1}$, exactly. This means that if N_A is expressed in reciprocal moles, its numerical value, $\{N_\mathrm{A}\}_{\mathrm{mol}^{-1}} = N_\mathrm{A}/\mathrm{mol}^{-1}$, is exactly equal to the gram-to-dalton mass-unit ratio, or, in terms of the kilogram:

$$\{N_\mathrm{A}\}_{\mathrm{mol}^{-1}} = (0.001\,\mathrm{kg})/\mathrm{Da}, \text{ exactly}, \qquad (6)$$

irrespective of how the kilogram and dalton are themselves defined. Equation (6) is a fundamental compatibility condition relating the numerical value of N_A (when N_A is expressed in reciprocal moles) to the kilogram and dalton.

2.2. The carbon-12-based dalton

Given the carbon-12-based definition of the dalton, $\mathrm{Da} = m_\mathrm{a}(^{12}\mathrm{C})/12$, equation (5) corresponds to the formal statement of the current definition of the mole, as seen by writing

$$\begin{aligned}\mathrm{mol} &= \{(0.001\,\mathrm{kg})/[m_\mathrm{a}(^{12}\mathrm{C})/12]\}/N_\mathrm{A}\\ &= (0.012\,\mathrm{kg})/[N_\mathrm{A} m_\mathrm{a}(^{12}\mathrm{C})]\\ &= 0.012 m(\mathscr{K})/M(^{12}\mathrm{C}),\end{aligned} \qquad (7)$$

where $m(\mathscr{K})$ is the mass of the International Prototype of the kilogram and $M(^{12}\mathrm{C})$ is the amount-specific mass of carbon 12. In current SI base units, both $m(\mathscr{K})$ and $M(^{12}\mathrm{C})$ have exact numerical values: $m(\mathscr{K}) = 1\,\mathrm{kg}$, exactly, and $M(^{12}\mathrm{C}) = 0.012\,\mathrm{kg\,mol}^{-1}$, exactly. The gram-to-dalton mass-unit ratio, $(0.012\,\mathrm{kg})/m_\mathrm{a}(^{12}\mathrm{C})$, is ‘the number of atoms in 0.012 kilogram of carbon 12,’ as used in the formal statement of the current definition of the SI mole [6].

2.3. The fundamental stoichiometric equations

Rewriting the amount-of-substance equation, (5), as

$$n(\mathrm{X}) = N(\mathrm{X})/(\mathrm{g}/\mathrm{Da})\,\mathrm{mol}, \qquad (8)$$

we can summarize the two fundamental stoichiometric equations, (2) and (8), in an easily comprehended dimensionless form, as follows:

$$m(\mathrm{X})/[A_\mathrm{r}(\mathrm{X})\,\mathrm{g}] = N(\mathrm{X})/(\mathrm{g}/\mathrm{Da}) = n(\mathrm{X})/\mathrm{mol}. \qquad (9)$$

Since g/Da is a known (albeit inexact) number—the current CODATA (2010) value [7] is 6.022 141 29(27) × 10^{23}—and for specified X, $A_\mathrm{r}(\mathrm{X})$ can be found from tables of relative atomic masses, given any one of $m(\mathrm{X})$, $N(\mathrm{X})$ or $n(\mathrm{X})$, we can find the other two from these two straightforward stoichiometric equations.

2.4. The proposed redefinitions of the mole and kilogram

With the proposed redefinitions of SI base units [1], the substance-mass equation, written in terms of the (redefined) gram, equation (2), remains the same. However, in terms of the redefined mole, the amount-of-substance equation is different from equation (8). In explicit-unit form, the proposed new mole definition would be

$$\mathrm{mol} = N^*/N_\mathrm{A}, \text{ exactly}, \qquad (10)$$

where N^* is an exact dimensionless constant. For seamless continuity with the current definition, this constant would be *fixed* at a value equal to the best estimate of g/Da at the time of transition to the new definitions, $t = T$:

$$N^* = (\mathrm{g}/\mathrm{Da})^*_T = 0.012/[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]^*_T, \text{ exactly}, \qquad (11)$$

where the subscript and asterisk indicate a fixed exact value of the quantity within the parentheses or brackets. It should be clear that the amount-specific mass of carbon 12, $M(^{12}\mathrm{C}) = N_\mathrm{A} m_\mathrm{a}(^{12}\mathrm{C}) = N^*[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]\,\mathrm{kg\,mol}^{-1}$, is then no longer an exact constant.

In terms of the redefined mole, the amount-of-substance equation, (3), then becomes

$$n(\mathrm{X}) = [N(\mathrm{X})/N^*][N^*/N_\mathrm{A}] = [N(\mathrm{X})/N^*]\,\mathrm{mol} \qquad (12)$$

or, in dimensionless form,

$$n(\mathrm{X})/\mathrm{mol} = N(\mathrm{X})/N^*. \qquad (13)$$

Compared with equations (9), the dimensionless stoichiometric equations, relating $m(\mathrm{X})$, $N(\mathrm{X})$ and $n(\mathrm{X})$, now have the more complicated form

$$m(\mathrm{X})/[A_\mathrm{r}(\mathrm{X})\,\mathrm{g}] = N(\mathrm{X})/(\mathrm{g}/\mathrm{Da}) = (1+\kappa)[n(\mathrm{X})/\mathrm{mol}], \tag{14}$$

where the term $(1+\kappa)$ represents an explicit molar mass *correction factor* [3], $(1+\kappa) = N^*/(\mathrm{g}/\mathrm{Da})$—since $N^*(= 0.012/[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]_T^*)$, an *exact* constant, is not equal to g/Da, which is the *inexact* quantity $0.012/[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]$. In fact,

$$N^*/(\mathrm{g}/\mathrm{Da}) = [m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]/[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]_T^* = \mathscr{R}_\mathrm{C}(t), \tag{15}$$

the ratio of the experimentally determined carbon-12 atomic mass, expressed in kilograms, to its fixed exact value set at the time of transition—an inexact factor, the estimated value of which will vary over time with CODATA adjustments of $m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}$ [8].

Although the correction factor was originally written explicitly as $(1+\kappa)$ in [3], this evidently seemed confusing to many people, so subsequent publications [4, 5] preferred to abandon the explicit correction factor and to redefine the so-called molar mass constant, M_u—currently, exactly equal to $1\,\mathrm{g\,mol^{-1}}$—as (the now *inexact* and *non-constant* quantity) $M(^{12}\mathrm{C})/12 = N^* m_\mathrm{a}(^{12}\mathrm{C})/(12\,\mathrm{mol})$, thereby replacing the quantity $(1+\kappa)\,\mathrm{g\,mol^{-1}}$. Using this, the dimensionless stoichiometric equations then become

$$\begin{aligned} m(\mathrm{X})/[A_\mathrm{r}(\mathrm{X})\,\mathrm{g}] &= N(\mathrm{X})/(\mathrm{g}/\mathrm{Da}) \\ &= [M(^{12}\mathrm{C})/(12\,\mathrm{g\,mol^{-1}})][n(\mathrm{X})/\mathrm{mol}], \end{aligned} \tag{16}$$

which, compared with equations (9), would undoubtedly be very confusing and extremely difficult to explain to beginning science students—who would (justifiably) want to know where the 'exotic looking' factor $M(^{12}\mathrm{C})/(12\,\mathrm{g\,mol^{-1}})$ comes from.

3. Redefining the dalton exactly in terms of the kilogram

The incompatibility requiring the correction factor in equation (16) is caused by setting the left-hand side of equation (6) equal to an exact constant without simultaneously setting the right-hand side equal to the same constant; in other words, by retaining the carbon-12-based dalton in conjunction with the fixed-N_A mole and fixed-h kilogram. Since equations (16) can be written as

$$m(\mathrm{X})/[A_\mathrm{r}(\mathrm{X})\,\mathrm{g}] = \mathscr{R}_\mathrm{C}(t)[N(\mathrm{X})/N^*] = \mathscr{R}_\mathrm{C}(t)[n(\mathrm{X})/\mathrm{mol}], \tag{17}$$

by dividing through by $\mathscr{R}_\mathrm{C}(t)$, we can rewrite this as

$$[m(\mathrm{X})/\mathrm{g}]/[\mathscr{R}_\mathrm{C}(t)A_\mathrm{r}(\mathrm{X})] = N(\mathrm{X})/N^* = n(\mathrm{X})/\mathrm{mol}. \tag{18}$$

The denominator of the left-hand term is, noting equation (11),

$$\begin{aligned} &\mathscr{R}_\mathrm{C}(t)A_\mathrm{r}(\mathrm{X}) \\ &\quad = \{[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]/[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]_T^*\} m_\mathrm{a}(\mathrm{X})/[m_\mathrm{a}(^{12}\mathrm{C})/12] \\ &\quad = m_\mathrm{a}(\mathrm{X})/[1/(1000N^*)\,\mathrm{kg}]. \end{aligned} \tag{19}$$

If we now redefine the dalton as

$$\mathrm{Da} = 1/(1000N^*)\,\mathrm{kg}, \text{ exactly}, \tag{20}$$

the corresponding relative atomic mass, using the redefined dalton, becomes

$$A_\mathrm{r}(\mathrm{X}) = m_\mathrm{a}(\mathrm{X})/\mathrm{Da} = m_\mathrm{a}(\mathrm{X})/[(1/1000N^*)\,\mathrm{kg}], \tag{21}$$

so that the stoichiometric equations now have the easily comprehended form

$$m(\mathrm{X})/[A_\mathrm{r}(\mathrm{X})\,\mathrm{g}] = N(\mathrm{X})/N^* = n(\mathrm{X})/\mathrm{mol}, \tag{22}$$

where, for a given X, $A_\mathrm{r}(\mathrm{X})$ is obtained from standard (comparatively low-precision) tables of relative atomic masses (which, as shown in the next section, will be unchanged from their current values) and N^* is an exactly known number (for example, using the currently best-known value, N^* would be exactly $6.022\,141\,29 \times 10^{23}$). Redefining the dalton in this compatible manner would seem to be a much better strategy than introducing confusing *ad hoc* inexact correction factors such as $(1+\kappa)$ or the proposed 'modified molar-mass constant'—simply for the sake of retaining the incompatible carbon-12-based dalton in defining relative atomic mass.

4. Decoupling the dalton from the carbon-12 reference mass

Since the redefined dalton would no longer be equal to $m_\mathrm{a}(^{12}\mathrm{C})/12$, it could not still be used for cataloguing nuclidic mass ratios of the form $R_\mathrm{n}^\mathrm{C}(\mathrm{X}) = 12\{m_\mathrm{a}(\mathrm{X})/m_\mathrm{a}(^{12}\mathrm{C})\}$—where the braces indicate direct measurement of the argument (for example, by mass spectrometry). Such ratios would simply be catalogued in terms of multiples of the 'carbon-12 reference mass,' perhaps requiring a new symbol such as, for example, $m_\mathrm{C} = m_\mathrm{a}(^{12}\mathrm{C})/12$.

Using the redefined dalton and $A_\mathrm{r}(\mathrm{X}) = m_\mathrm{a}(\mathrm{X})/\mathrm{Da}$, the relative atomic mass is related to $R_\mathrm{n}^\mathrm{C}(\mathrm{X})$ by

$$A_\mathrm{r}(\mathrm{X}) = \{[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]/[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]_T^*\} R_\mathrm{n}^\mathrm{C}(\mathrm{X}); \tag{23}$$

so, since $[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]_T^*$ is an exact constant and nuclidic mass ratios are known to extremely high precision, the relative standard uncertainty of a given relative atomic mass (using the redefined exact dalton) will be dominated by that of the carbon-12 atomic mass measured in kilograms, $u_\mathrm{r}[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]$. But, with the fixed-$h$ kilogram, the latter will be of order 10^{-9} or less [1, 4]—far more precise than anything needed for stoichiometric calculations. To the precision used in practice (usually not more than seven significant figures), there would not be any changes in the numerical values of relative atomic masses, as defined by equation (21), from their current values—ever!

5. The alternative carbon-12-based kilogram

It should perhaps be mentioned that a much more obvious compatible strategy would be to keep the carbon-12-based dalton with an exact-N^* mole, and redefine the kilogram in a different way by setting $\mathscr{R}_\mathrm{C}(t)$ in equation (15) exactly equal to 1. Since $[m_\mathrm{a}(^{12}\mathrm{C})/\mathrm{kg}]_T^*$ is a constant, equations (11) and (15) imply that the kilogram would then be defined as

$$\mathrm{kg} = (1000N^*/12)m_\mathrm{a}(^{12}\mathrm{C}), \text{ exactly}. \tag{24}$$

The dalton is then exactly related to the kilogram as in equation (20), and relative atomic masses, $m_a(X)/\mathrm{Da}$, are identical to directly measured nuclidic mass ratios referenced to carbon 12, $12\{m_a(X)/m_a(^{12}C)\}$, which means that nuclidic masses can now be expressed directly in terms of the carbon-12-based kilogram to extremely high precision.

Using the current best estimate of N^*, this kilogram definition would be

$$\mathrm{kg} = 5.018\,451\,075 \times 10^{25} m_a(^{12}C), \text{ exactly.} \tag{25}$$

Although it seems likely that students and non-metrologist members of the wider scientific and user community would understand and prefer this definition in terms of a real physical atomic mass [9, 10], the CGPM, on the basis of a proposal from the CCU, approved by the CIPM, has endorsed the less easily comprehended fixed-Planck-constant definition—since, in combination with the proposed redefinition of the ampere that fixes the numerical value of the elementary charge, e, this guarantees that certain quantum-electronic parameters (specifically, the von Klitzing constant, $R_K = h/e^2$, and the Josephson constant, $K_J = 2e/h$) and a number of related quantities will have exact numerical values [3].

The Planck constant and the atomic mass of carbon 12 are related by

$$h/m_a(^{12}C) = (c_0/2)(1/R_\infty)[m_e/m_a(^{12}C)]\alpha^2, \tag{26}$$

where c_0 is the vacuum light speed, R_∞ is the Rydberg constant, m_e is the electron mass and α is the fine-structure constant [3]. The term $c_0/2$ is exact; the currently known [7] relative standard uncertainties of the other quantities are $u_r(R_\infty) = 5.0 \times 10^{-12}$, $u_r[m_e/m_a(^{12}C)] = 4.0 \times 10^{-10}$ and $u_r(\alpha) = 3.2 \times 10^{-10}$. The combined uncertainty of the right-hand side of equation (26) is therefore

$$\begin{aligned} u_r(\mathrm{RHS}) &= [(5.0 \times 10^{-12})^2 + (4.0 \times 10^{-10})^2 \\ &\quad + (2 \times 3.2 \times 10^{-10})^2]^{1/2} \\ &= 7.5 \times 10^{-10}. \end{aligned} \tag{27}$$

So if the kilogram were to be redefined in terms of the carbon-12 atomic mass as in equation (24) together with a fixed-e ampere, the Planck constant and the von Klitzing and Josephson constants would not be exactly known; but they would have relative standard uncertainties of, initially, only 7.5×10^{-10}; and these uncertainties would decrease even further as more precise values of the electron mass (in terms of the carbon-12-based kilogram) and the (dimensionless) fine-structure constant became available.

Some chemical metrologists have argued strongly in favour of retaining the current definition of the mole, i.e. keeping $M(^{12}C)$ fixed at exactly $12\,\mathrm{g\,mol^{-1}}$—regardless of how the kilogram is redefined [11]. In this case, if the fixed-h kilogram were to be adopted (while retaining the carbon-12-based dalton), N_A, being equal to $(\mathrm{g/Da})\,\mathrm{mol^{-1}}$, would not have an exact value. However, with the carbon-12-based kilogram (and dalton), fixing $M(^{12}C)$ would mean that the Avogadro constant (expressed in reciprocal moles) would have a fixed exact value; i.e. equivalent to a 'fixed-N_A' mole.

6. Summary

It is important to emphasize at the outset that, as has been shown, the fundamental definition of the macroscopic unit for amount of substance states that the mole must be exactly proportional to the gram-to-dalton mass-unit ratio. In symbols: $\mathrm{mol} = (\mathrm{g/Da})/N_A$, exactly, where the Avogadro constant, N_A, *defines* the physical quantity amount of substance, $n(X)$, in terms of the total number of entities, $N(X)$, i.e. $n(X) = N(X)/N_A$. The *only* defined property of the Avogadro constant is that it is indeed a constant, independent of the substance involved, with the dimension of reciprocal amount of substance. As shown in section 2.1, when N_A is expressed in reciprocal moles, it must have the numerical value $\{N_A\}_{\mathrm{mol^{-1}}} = (0.001\,\mathrm{kg})/\mathrm{Da}$, exactly. This cannot be stressed too strongly: the numerical value of the Avogadro constant (when N_A is expressed in reciprocal moles) *is synonymous with* the gram-to-dalton mass-unit ratio—the ratio of two man-made mass units, *chosen* appropriately (but arbitrarily) for the macroscopic and atomic scales, respectively. This numerical value of N_A cannot be set at any other value independently of this mass-unit ratio without creating a fundamental incompatibility.

It should now be obvious that to propose that $\{N_A\}_{\mathrm{mol^{-1}}}$ be set at an exact value, N^*, is logically equivalent to proposing that g/Da be set exactly equal to N^*, or, equivalently, that $\mathrm{Da} = 1/(1000N^*)\,\mathrm{kg}$, exactly. Unfortunately, the architects of the proposed new SI definitions seem to have ignored the fundamental origin of the mole that specifies $\mathrm{mol} = (\mathrm{g/Da})/N_A$, exactly, and instead have treated the Avogadro constant as if it were an *independent* quantity, proposing that $\{N_A\}_{\mathrm{mol^{-1}}}$ be set at an exact value without redefining the dalton compatibly in terms of the kilogram. The resulting incompatibility requires a 'patch-up' strategy involving a correction factor such as the $(1 + \kappa)$ factor originally proposed—now evidently to be replaced by $M(^{12}C)/(12\,\mathrm{g\,mol^{-1}})$. This type of *ad hoc* procedure is not appropriate for a twenty-first-century redefinition of SI units. To predict that this would likely result in untold further confusion within stoichiometry and thermodynamics would seem to be a serious understatement.

There are three possibilities for compatible redefinitions of the mole, kilogram and dalton.

1. The kilogram is redefined exactly in terms of the carbon-12 atomic mass, in which case the (current) carbon-12-based dalton is compatible with a 'fixed-N_A' mole and $M(^{12}C)$ remains equal to $12\,\mathrm{g\,mol^{-1}}$, exactly [10].
2. With any other (i.e. non-carbon-12-based) kilogram definition, the carbon-12-based dalton and the current definition of the mole are retained, fixing $M(^{12}C)$; in this case (as currently), g/Da ($\equiv \{N_A\}_{\mathrm{mol^{-1}}}$) does not have an exact value [11].
3. Again, with a non-carbon-12-based kilogram, g/Da is set at a fixed value, thereby fixing $\{N_A\}_{\mathrm{mol^{-1}}}$ (i.e. giving a 'fixed-N_A' mole). As discussed here, this would require decoupling the redefined (exact) dalton from the (inexactly known) carbon-12 reference mass used for cataloguing nuclidic mass ratios to high precision; and it would require distinguishing 'relative atomic mass'

as used in stoichiometry (using the exact dalton) from 'nuclidic mass ratio' (using the carbon-12 reference mass). These quantities are already catalogued to widely differing precisions; this formal separation would require only minimal changes in terminology and notation. Implementation of the changes would, of course, require careful coordination between international standards bodies such as IUPAP and IUPAC, particularly the latter's Commission on Isotopic Abundances and Atomic Weights.

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