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COMMENT AND REPLY

Comment on:
"Nominal Mass?" by Athula B. Attygalle and Julius Pavlov, *J. Am. Soc. Mass Spectrom.* 28, 1737-1738 (2017)

A recent correspondence [1] suggests that the current International Union of Pure and Applied Chemistry (IUPAC) recommendation [2] for the definition of *nominal mass* is flawed and should be expanded so that all possible isotope combinations for a molecule or ion can be assigned a whole number mass. The authors propose a revised definition for nominal mass as "the sum of the unified mass scale-based integer masses of its constituent protons and neutrons." This comment is aimed at showing that nominal mass is well defined and widely used and is an essential concept in mass spectrometry. As an alternative to redefining nominal mass, it is suggested that integer mass, defined as the sum of the mass numbers of the elements comprising a molecular ion or molecule, be used.

The nominal mass of an ion, molecule, or atom is defined as the sum of the isotope mass of the most abundant isotopes of the constituent elements rounded to the nearest integer [2]. This definition is widely accepted in the mass spectrometry community as exhibited by its consistent use in articles [3, 4], glossaries [5, 6], reference books [7, 8], and textbooks [9–12]. The nominal mass can be easily and unambiguously found by summing the integer mass of the appropriate constituent atoms, which is equivalent to summing their mass numbers (nucleon numbers) [13]. The most abundant isotope can be obtained using tables that are regularly reported by the International Union of Pure and Applied Chemistry (IUPAC) Commission on Isotopic Abundances and Atomic Weights (CIAAW) [14]. There are no examples of atoms for which the observed range of natural variations would change the mass number of the most abundant isotope [14, 15]. Although worded in different ways, the published definitions of nominal mass are consistent. Some note explicitly that only naturally occurring stable isotopes be considered in determining the nominal mass [7, 10]. Thus, elements with no stable isotope have no defined nominal mass just as they do not have a defined standard atomic weight [16]. The definition provided by the Committee on Measurements and Standards of the American Society for Mass Spectrometry is consistent with those above [5].

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The definition of nominal mass parallels that of monoisotopic mass, which is defined as the exact mass of an ion or molecule calculated using the mass of the most abundant isotope of each element [2]. The exact mass of a molecule or ion is the sum of the masses of its constituent isotopes. Thus, every molecule has a single monoisotopic mass as well as a single nominal mass. Both concepts are useful and their definitions rely on the concept of most abundant isotope.

The term integer mass is currently used in the way that the authors suggest for their revised definition of nominal mass [10, 11]. The integer mass of an atom or atomic ion is the mass number of the particular isotope of an element with the dimension of mass in unified atomic mass units. The integer mass of molecule or molecular ion can be defined as the sum of the integer masses of the constituent atoms. Nominal mass is then the integer mass obtained from the most abundant stable isotopes of the constituent elements. This pair of definitions is parallel to those for exact mass and monoisotopic mass; the set of definitions is indicated in Table 1. Note that integer and nominal mass as well as exact and monoisotopic mass have the dimension mass.

There are instances in the literature where nominal mass has been used with the meaning of unit mass or integer mass [17–20]. The terms nominal *m/z* [10, 12] and nominal resolution [21, 22] have also been used where "nominal" indicates "integer" rather than integer mass of the most abundant isotope. In these cases, using the terms integer mass, integer *m/z* (or unit *m/z*), and integer resolution (or unit resolution), respectively, will remove the ambiguity.

In summary, Attygalle and Pavlov raise a valid point regarding the lack of a term to describe the mass obtained by summing of the mass numbers of the constituent elements of a molecular ion or molecule with an arbitrary isotopic composition. Rather than generalize the term nominal mass, the use of the term integer mass is suggested.

Table 1.. Proposed Definition for Integer Mass, Nominal Mass, Exact Mass, and Monoisotopic Mass

	Element	Molecule or ion
Integer mass	Mass number	Sum of the integer masses of the constituent atoms
Nominal mass	Mass number of the most abundant stable isotope	Sum of the nominal masses of the most abundant stable isotopes
Exact mass	Atomic mass	Sum of the atomic masses of constituent atoms
Monoisotopic mass	Atomic mass of the most abundant stable isotope	Sum of the atomic masses of the most abundant stable isotopes

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