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MASS SPECTROMETRY

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Language of Mass Spectrometry

Although it is important to be conversant in the language and symbolism of mass spectrometry, the literature is full of errors, mistakes and poor expressions. The focus of this workshop is to start a dialog and find ways to express ourselves professionally to avoid confusions. Consider “Nominal Mass” as an example. It is a term technical widely used in mass spectrometry textbooks and research papers. According the authoritative body for recommending and standardizing nomenclature for chemists the International Union of Pure and Applied Chemists (IUPAC), the term “nominal mass” is defined as the “mass of a molecular ion or molecule calculated using the isotope mass of the *most abundant* constituent element isotope of each element rounded to the nearest integer value and multiplied by the number of atoms of each element.” Albeit popular, this definition is flawed. In a recent correspondence to the editor of the Journal of the American Society for Mass Spectrometry (DOI: 10.1007/s13361-017-1647-6), it was point out that this definition would impl, for example that the nominal mass of the element xenon would have to be chosen as 132. Although xenon is mixture of many isotopes, the ¹³²Xe is chosen to represent the whole group because it the most abundant isotope of the element, despite the fact that it is only a fraction of a per cent more abundant than its rival ¹²⁹Xe. By the same definition, all man-made artificial elements should not be assigned a nominal mass because their natural abundance is zero. Furthermore, any isotopically labeled compound cannot (or must not) be assigned a nominal mass when the enriched isotope happens not to be the naturally most abundant one.

Biography

Athula Attygalle is a Professor at Stevens Institute of Technology, USA. He became the Director at Cornell University in 1991. After 12 years, he became a Professor at Stevens Institute of Technology in Hoboken, in 2001. He has published over 200 papers in reputed journals and holds five US patents

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