Subcommittee on Natural Assessment of Fundamental Understanding of Isotopes of IUPAC

Accomplishments 2020–2021

by

Norman E. Holden, Chair

The Subcommittee did not hold any meetings in 2020 or 2021.

By December 14, 2019, it was recognized that *Pure and Applied Chemistry* was not going to publish the outcomes of IUPAC project 2015-030-2-200 on providing choices to the Commission for expression of uncertainty of standard atomic weights that would be in compliance with the GUM (Guide for Expression of Uncertainty in Measurement). The outcomes of this effort were provided to the IUPAC Secretariat and can be found online at https://iupac.org/wp-content/uploads/2020/05/SNAFUI_2017report.pdf.

The Subcommittee Chair (Dr. Norman E. Holden) suggested that we should redirect our efforts and publish a manuscript in another journal that might garner a wider audience, which was not familiar with *Pure and Applied Chemistry* and IUPAC. The editor of *Rapid Communications and Mass Spectrometry* was contacted to see if he would be receptive to an article tentatively titled "The Making of a Standard Atomic Weight—An Exercise in Consensus" that would address the following questions:

- How are new standard atomic-weight values determined, and what are the guidelines for updating them?
- What are the uncertainties on standard atomic-weight values—standard uncertainties or expanded uncertainties?
- What is the new format for expressing standard atomic-weight values and their uncertainties to make it clear that they are expanded uncertainties?
- Why do 13 elements now have standard atomic-weight values expressed as intervals?
- When an element has a standard atomic-weight value expressed as an interval, what single value is provided for use in education, commerce, and trade?
- Why do 34 elements have no standard atomic weight?

The editor was strongly supportive of submission of such an article.

An article titled "The Table of Standard Atomic Weights—an exercise in consensus" was prepared by Tyler B. Coplen, Norman E. Holden, Tiping Ding, Harro A. J. Meijer, Jochen Vogl, and Xiangkun Zhu. Excluding the abstract, introduction, and conclusions, the main sections of the article were:

- 1. Components of the Commission's Table of Standard Atomic Weights (3pages)
 - a. History and importance of annotations and footnotes
 - b. Subcommittee on Natural Isotopic Fractionation (SNIF)

- c. Expression of standard atomic weight values as intervals
- d. Conventional atomic weight values
- 2. The process of revising a standard atomic weight value (3 pages)
- 3. Precision versus reliability of standard atomic weights (1.5 pages)

The last paragraph of the abstract highlights the benefits of the process used for updating standard atomic weight values, and it is highly complementary of IUPAC and the Commission. It states:

"Not only has the Commission shielded users of the TSAW and TICE from unreliable measurements that appear in the literature as a result of unduly small uncertainties, but the aim of IUPAC has been fulfilled by which any scientist, taking any natural sample from commerce or research, can expect their sample atomic weight to lie within $A_r(E) \pm$ its uncertainty almost all of the time."

This article was accepted by *Rapid Communications and Mass Spectrometry* and appeared online June 19, 2020. This article is the only peer reviewed publication that documents three possible formats developed under IUPAC project 2015-030-2-200 to eliminate the noncompliance of expression of standard atomic weight uncertainty with the GUM.