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Forecast of Standard Atomic Weights for the Mononuclidic Elements – 2011

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Forecast of Standard Atomic Weights for the Mononuclidic Elements – 2011

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Introduction

The history of the atomic weights and standard atomic weight values over the last half century was reviewed some few years ago[1]. The chemist's early values of atomic weights were based upon either the hydrogen = 1 scale or the oxygen = 100 scale. In more recent times, the scale of elemental oxygen = 16 was used. This latter (chemist) scale differed from the physicist's scale of the nuclide ^{16}O = 16, when Giaugue and Johnson[2, 3] reported that oxygen contained small amounts of the isotopes of mass 17 and mass 18. When Dole[4] reported the variation in the oxygen atomic weight in water versus in air, this determination implied that there was a variation in the isotopic composition of oxygen and it meant that these two scales had a small but a variable difference. This relatively small but basic difference would persist for the next quarter of a century.

Nier[5] proposed ^{12}C = 12 as a reference species for a new unified scale. In 1959 at the Munich, Germany General Assembly of the International Union of Pure and Applied Chemistry (IUPAC), the Atomic Weights Commission recommended the adoption of ^{12}C = 12 as a reference for a new scale, if the International Union of Pure and Applied Physics (IUPAP) made a similar adoption. IUPAP took this action at their 1960 Ottawa, Canada General Assembly.

A new Atomic Mass Table (based on the new mass scale with ^{12}C = 12) was published in 1960[6]. The consistent set of nuclidic masses was computed with least squares methods from all significant experimental data for the mass numbers less than 200. There were not enough experimental data to perform a least squares fit for the data above "A" > 200. For the mass region from samarium to thallium, Nier[7] had just published new mass data that became available too late to allow its use in the 1960 Atomic Mass Table publication. Cameron and Wichers' Atomic Weight report[8] used the new Nier mass data with the 1960 Mass Table as the basis for the 1961 Atomic Weights revision. Subsequent mass tables, all based on the ^{12}C = 12 scale, were updated in 1964[9], 1971[10], 1977[11], 1983[12], 1993[13] and 2003[14]. These Atomic Mass Tables have been published over the past half-century with a frequency of about six to seven years earlier on and more recently with about a ten year frequency. The next publication of the Atomic Mass Table is scheduled for late in 2012 or early in 2013.

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In this short report, I will provide an early warning about potential changes to the standard atomic weight values for the twenty mononuclidic and the so-called pseudo-mononuclidic (^{232}Th and ^{231}Pa) chemical elements due to the estimated changes in the mass values to be published in the next Atomic Mass Tables within the next two years. There have been many new measurements of atomic masses, since the last published Atomic Mass Table. The Atomic Mass Data Center has released an unpublished version of the present status of the atomic mass values as a private communication[15]. We can not update the Standard Atomic Weight Table at this time based on these unpublished values but we can anticipate how many changes are probably going to be expected in the next few years on the basis of the forthcoming publication of the Atomic Mass Table.

I will briefly discuss the procedures[16] that the Atomic Weights Commission used in deriving the recommended Standard Atomic Weight values and their uncertainties from the atomic mass values.

I will also discuss some concern raised about a proposed change in the definition of the mole. The definition of the mole is now connected directly to the mass of a ^{12}C isotope (which is defined as 12 exactly) and to the kilogram. A change in the definition of the mole will probably impact the mass of ^{12}C.

The Commission's Technical Procedure for Mononuclidic Elements

In the 1961 Element by Element review of atomic weight values by Cameron and Wichers[8], the Commission indicated that the atomic weight values for the mononuclidic elements were no longer based on chemical determinations but were based on nuclidic mass data derived from physical measurements.

Since isotopic abundance values for mononuclidic elements are 100% exactly, atomic weight values should agree with the atomic mass values. In practice, approximately the last two significant digits were deleted from the atomic mass value to provide confidence in the atomic weight values. This procedure allowed for the uncertainty due to possible minor nuclides of an element that might be discovered at a very low abundance level. The nuclide ^{180}Ta had just recently been discovered. It was pointed out by Aaldert Wapstra, the author of the Atomic Mass Tables, that the quoted uncertainties referred to the consistency of each atomic mass value relative to its neighboring nuclides and was not related to uncertainties in the quoted mass relative to the mass standard, ^{12}C.

At the New York IUPAC General Assembly in 1951, the Commission[17] attached a range of ± 0.003 to the atomic weight of sulfur in order to indicate the range of values that may apply to sulfur from different natural sources. This range was due to the analysis of the natural variations in the abundance ratios of isotopes from a report by Marble[18].

Finally in 1969, the Commission[19] introduced long-lived nuclides into Atomic Weights Table, as well as uncertainty values for the reported atomic weights. Quoted uncertainties were restricted to values of either ±1 or ± 3, which indicated the relative confidence in the atomic weight values presented. The values of the atomic weights for the mononuclidic elements were rounded up to a smaller number of significant digits until the estimated uncertainty in the values was less than or equal to ±1 in the last digit.

Over the years, the Commission gradually decided that the most accurate atomic weight values should be transmitted to the users independednt of whether that accuracy was required for contemporary experiments or not. In the 1983 Atomic Weights report[20], in keeping with this decision to provide the most accurate values, the uncertainty values assigned to elemental atomic weight values were expanded to include all digits. The older and long standing policy on the mononuclidic elements still used a multiplicative factor of six on the atomic mass uncertainty. However, the uncertainty values which resulted were now rounded up to the next single digit instead of being rounded up to ±1.

Impact on the Atomic Mass Standard of a Redefinition of the Mole

At present, the mass of ^{12}C is an absolute invariant of nature. In the proposed new definition of the mole, the value of Avogadro's constant would become the fixed invariant of nature and the mass of ^{12}C would be determined experimentally. Since the atomic weight values are currently defined on the basis of $^{12}C = 12$ exactly, a slight change in the mass of ^{12}C would have an impact on each atomic weight value. In addition, the uncertainty that would be introduced for the mass of ^{12}C would now have to be incorporated into the uncertainty for every other atomic mass. For the majority of chemical elements, the uncertainty in the isotopic composition would greatly outweigh any small change in the atomic mass of ^{12}C. However, this is not true for the twenty-two mononuclidic or pseudo-mononuclidic elements.

Discussion

On the basis of the recent unpublished atomic mass data and under present Commission's procedures for handling uncertainties, there would be no change in either the value or the uncertainty of the atomic weight for the two pseudo-mononuclidic elements. For the other twenty true mononuclidic elements, the uncertainty would have changed for half of these elements (a total of ten) up to the present time, with a total of nine decreases in the uncertainty and one increase in the uncertainty.

Overall, for these twenty mononuclidic elements, five atomic weight values would have increased, eight atomic weight values would have decreased and seven of the values would have stayed the same. Of the latter seven unchanged values, five would have identical values and uncertainties, while the other two identical values would have an uncertainty that went up for one element and down for the second element.

There are a significant number of changes to the atomic weight values and uncertainties under the present Commission's procedures. However, if these procedures should be reevaluated on the basis of some previous comments from Audi on the reliability of the uncertainties in the atomic masses, as well as a reexamination of the effect of a change in the contemplated definition of the mole, there could be even more changes in the atomic weights to consider when the new atomic mass table is released in a few years.

Conclusions

This report summarizes some of the anticipated changes in the atomic weight values and uncertainties of the mononuclidic elements. It is based on a short review of unpublished information that has recently been made available. It applies the Commission's technical rules to this latest information of the atomic mass table and discusses potential changes in the values of the Standard Atomic Weights. The effect on atomic weights from a change in the definition of the mole should be examined. It is recommended that a Project be initiated to review the impact on the Standard Atomic Weight values and uncertainties in advance of the anticipated new Atomic Mass table in the next two years.

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