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Standard Atomic Weight Values for the Mononuclidic Elements - 2001

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Atomic Mass Evaluations have had a major impact on the values of the atomic weights for the twenty mononuclidic elements plus two elements, Thorium and Protactinium, which have no stable nuclides but a characteristic terrestrial isotopic composition. This paper reviews the history of the atomic weight values of these elements in the years, since the reference mass standard changed from ^{16}O to ^{12}C. There is a problem for Thorium, which is considered to have an abundance value of 100%, but is not treated as such in the Standard Atomic Weights' Table. Recommendations for handling the Standard Atomic Weight values for 2001 are presented.

I. Introduction

Since the time of Dalton, the values of the atomic weights of the chemical elements have varied due to the `atomic scale', i.e., the element used as a reference and its value. In the early years of the past century[1], the reference for the atomic weight scale stabilized at oxygen ≡ 16.

In 1929, Giaugue and Johnson[2,3] discovered that oxygen contained small amounts of isotopes of mass 17[3] and mass 18[2]. The chemist's scale of O = 16 now differed from the physicist's scale of $^{16}O \equiv 16$. In 1935, Dole[4] reported the variation in the oxygen atomic weight in water versus air. This implied variation in the isotopic composition of oxygen meant that the two scales had a small but variable difference. This difficulty persisted for a quarter century.

In the late 1950's, Nier[1] proposed $^{12}C \equiv 12$ 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

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Chemistry (IUPAC), the Atomic Weights Commission recommended adoption of $^{12}C \equiv 12$ 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 revised Atomic Mass Table, based on the new mass scale with $^{12}C \equiv 12$, was published in 1960[5] and used as the basis for the 1961 Atomic Weight revision by Cameron and Wichers[6]. 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 also used the Nier data in conjunction with the 1960 Mass Table. Subsequent mass tables, all on the $^{12}C \equiv 12$ scale, were updated in 1964[8], 1971[9], 1977[10], 1983[11], 1993[12] and 1995[13] and 1997[14].

In this report, I will trace the impact on the standard atomic weight values for the twenty-two mono-nuclidic and pseudo-mono-nuclidic chemical elements due to the mass values in the various Atomic Mass Tables over time. I will also discuss the procedures of the Atomic Weights Commission[15] in deriving the recommended Standard Atomic Weight values and their uncertainties from atomic mass values.

II. The Commission's Technical Procedure for Mono-Nuclidic Elements

In the 1961 Element by Element review of atomic weight values by Cameron and Wichers[6], the Commission indicated that the atomic weight values for the mono-nuclidic elements were no longer based on chemical determinations but were based on nuclidic mass data derived from physical measurements.

Since the isotopic abundance value for mononuclidic elements was 100%, the atomic weight value should agree with the atomic mass value. 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 other possible minor nuclides of the element that might be discovered at a very low abundance level. 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.

Midway through the decade, uncertainties began to be included with some of the atomic weight values, which were derived from "absolute" measurements of the isotopic abundance as those particular elements were updated in the biennial review. Finally in 1969, the Commission introduced long-lived nuclides into the Atomic Weight's Table, as well as uncertainty values for the reported atomic weights. The quoted uncertainties were restricted to values of ± 1 or ± 3, which indicated the relative confidence in the atomic weight values presented. However, these two uncertainty values were only provided for the poly-nuclidic elements. The available precision for the mono-nuclidic elements was considered to be in excess of the practical interests of chemical users of the Atomic Weight Tables. These values were rounded up to a smaller number of significant digits until the estimated uncertainty was less than or equal to ± 1.0 in the last digit.

The ±3 option was not applied to these mono-nuclidic elements.

Over the years, the Commission gradually decided that the most accurate atomic weight values should be transmitted to the users independent of whether that accuracy was required for contemporary experiments or not. In 1983 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, i.e., the available uncertainties went from restricted values of ±1 and ±3 to include all digits from ±1 up to ±9. The long standing policy on the mono-nuclidic elements still used a multiplicative factor of six on the atomic mass uncertainty. However, the uncertainty value which resulted was now rounded up to the next single digit instead of being rounded up to ±1 in the preceding digit of the atomic weight value.

As mentioned earlier, long-lived nuclides were included in the Tables beginning in 1969. This practice continued until 1981. Although these nuclides did not appear in the Atomic Weight Table in 1983, ^{231}Pa alone was reintroduced in 1985 and continues to be included in the present Tables.

III. Development of the Standard Atomic Weight Values and Uncertainties

For the change in the Atomic Weight scale in 1961, Cameron and Wichers made use of the 1960 Atomic Mass Table, as well as the 1960 atomic mass measurements of Nier. As far as the mononuclidic elements were concerned, ^{231}Pa was not considered at that time so there were only twenty-one elements involved. This is the standard twenty mono-nuclidic elements and thorium. There was no entry for ^{169}Tm in the 1960 Atomic Mass Table. The mass values for it, as well as for ^{165}Ho and ^{197}Au were taken from Nier's paper. Uncertainties were not considered at that time. The policy of the Commission was to take the value in the Atomic Mass Table and reduce the number of significant digits, until the Commission felt confident in the value presented. Later, a more consistent and defensible policy was adopted. The published uncertainty on the masses in the Atomic Mass Table was multiplied by a factor of six and then rounded up to ±1 in the preceding digit.

If this more consistent policy had been adopted in the case of the 1961 Atomic Weight Table, this policy would work for the three Nier mass values and ten other masses from the 1960 Mass Table. However, an additional digit was eliminated in the case of ^{9}Be, ^{19}F, ^{23}Na, ^{27}Al, ^{31}P and ^{45}Sc. In addition, an extra digit was included in the case of ^{75}As and ^{159}Tb. In the 1961 Atomic Weight Table, no uncertainties had as yet been listed for any of the elements. The results for the 1960 and 1964 Atomic Mass Tables and for the 1961 and the 1969 Atomic Weight Tables are presented in Table I.

The Atomic Mass Table was next updated in 1964[8] but the Atomic Weights Commission did not make use of this updated Atomic Mass Table until the 1969 Atomic Weights meeting. By that time, preliminary results were already available for the 1971 Atomic Mass Table[9]. In the Atomic Weights Table for 1969, entries were added for the longest lived nuclides of neptunium, protactinium, actinium and radium, as mentioned above. Applying the consistent Commission policy to the 1969 Atomic Weights Table, in the case of four elements (^{19}F, ^{23}Na, ^{27}Al and ^{31}P), an additional digit was eliminated from the atomic weight value, compared to the application of the uncertainty rule to the Atomic Mass Table. For three other elements (^{133}Cs, ^{165}Ho and ^{209}Bi), the final digit was incorrect compared to the Atomic Mass Table value for those elements. With the publication of the 1971 Atomic Mass Table, these seven problem elements were corrected in the 1971 Atomic Weights Table.

In 1975, Smith and Wapstra[16] published new mass data on ^{19}F, which led to a lower uncertainty. This lower uncertainty allowed the Commission to apply the technical policy and update the atomic weights value by adding an additional digit. The results for the 1971 and 1977 Atomic Mass Tables and for the 1971 and 1977 Atomic Weight Tables are presented in Table II.

In 1983, Wapstra and Audi[11] updated the Atomic Mass Table, which was published in 1985. The use of the Commission's policy for the 1983 Atomic Mass Table agrees with the Atomic Weights Table, except for the case of thorium. For thorium, it was argued that Ionium (^{230}Th) was often found in thorium samples. The range in the isotopic composition values for Thorium samples had a low value of 1.7 parts-per-million (ppm) up to a high value of 15.7 ppm. As a result, the number of significant digits in the Thorium atomic weight value was restricted to those previously quoted.

In 1993, Audi and Wapstra[12] published a new Atomic Mass Table. Once again, the application of the technical procedure to the Atomic Mass Table values result in the values presented in the Atomic Weight Table, except for Thorium. The value for Thorium remains the same. The results for the 1983 and 1993 Atomic Mass Tables and for the 1985 and 1995 Atomic Weights Table are presented in Table III.

In 1995 and 1997, Audi and Wapstra[13,14] published articles with an update to the 1993 Atomic Mass Table. The results of the 1993 and 1995 Atomic Mass Tables and the 1995 Atomic Weights Table and the recommendation from the application of the Commission's policy to the 1995 Atomic Mass update are presented in Table IV. There are a number of small differences in the last digit of the atomic weight value or in the uncertainty or both.

IV. Discussion

In the various Tables, I, II, III and IV, the results for the Atomic Mass Tables and the Atomic Weight Tables can be compared. It will be noticed that there is a increase of one in the last digit of the Atomic Weight value for both ^{31}P and for ^{55}Mn. There is an additional digit in the Atomic Weight value and a change in uncertainty uncertainty value for ^{27}Al. These changes are minor and might conceivably change back in an updated mass table for ^{31}P and ^{55}Mn. However, there is a major inconsistency with the treatment of Thorium. In the Atomic Weight Table, thorium is considered to be long-lived with a characteristic isotopic composition. The amount of ^{230}Th in terrestrial thorium has been seen above to vary from 1.7 ppm to 15.7 ppm. In the Commission's publications of the Table of Isotopic Composition, thorium has always been quoted as mono-nuclidic, i.e., consisting of 100% of ^{232}Th. If this is the case, then there should be additional digits quoted for the atomic weight value. The Commission's publications have been inconsistent since

1985. The Commission should review this situation and make a decision on the quoted isotopic abundance value or on the quoted atomic weight value as given in the Commission's publication.

V. Conclusion

When the policy for determining the atomic weight values for the mononuclidic elements was changed some decades ago, it was argued that new mass tables would only be produced about once a decade. This has generally been consistent with recent experience since that time. The present plans are for a new update in the Atomic Mass Table within the next year or two. I would recommend that no changes be made at this time. However, the Commission's procedure should be systematically applied to the new Table and the resulting values incorporated into the next Standard Atomic Weight Table.

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VII. References

1. N.E. Holden, "The International Commission on Atomic Weigfhts - An Early Historical Review", Chemistry International 6 (1) 5-12 (1984).
2. W.F. Giaugue and H.L. Johnson, Nature (London) 123 318 (1929) and J. Am. Chem. Soc. 51 1436-1441 (1929).
3. W.F. Giaugue and H.L. Johnson, Nature (London) 123 813 (1929) and J. Am. Chem. Soc. 51 3528-3534 (1929).
4. M. Dole, J. Am. Chem. Soc. 57 2731 (1935).
5. F. Everling, L.A. König, J.H.E. Mattauch and A.H. Wapstra, Nucl. Phys. 18 529-569 (1960).
6. A.E. Cameron and E. Wichers, J. Am. Chem. Soc. 84 4175-4197 (1962).
7. V.B. Bhanot, W.H. Johnson, Jr. and A.O.C. Nier, Phys. Rev. 120 235-251 (1960).
8. J.H.E. Mattauch, W. Thiele and A.H. Wapstra, Nucl. Phys. 67 1-31 (1965).
9. A.H. Wapstra and N.B. Gove, Atomic Data Nucl. Data Tables 9 265-468 (1971).
10. A.H. Wapstra and N.B. Gove, Atomic Data Nucl. Data Tables 19 175-297 (1977).
11. A.H. Wapstra and G. Audi, Nucl. Phys. A432 1-54 (1985).
12. G. Audi and A.H. Wapstra, Nucl. Phys. A565 1-65 (1993).
13. G. Audi and A.H. Wapstra, Nucl. Phys. A595 409-480 (1995).
14. G. Audi, O.Bersillon, J. Bhachot and A.H. Wapstra, Nucl. Phys. A624 1-124 (1997).
15. J.R. De Laeter, Technical Booklet, 5th Edition (unpublished), IUPAC Commission on Atomic Weights and Isotopic Abundances, May 1999.
16. L. Smith and A.H. Wapstra, Phys. Rev. C11 1392-1400 (1975).

Table I. Atomic Mass and Atomic Weight Values - 1960, 1969

Nuclide	1960 At. Mass	1961 At. Weight	1964 At. Mass	1969 At. Weight
^{9}Be	9.0121858(9)	9.0122	9.0121855(10)	9.01218
^{19}F	18.9984046(7)	18.9984	18.9984046(8)	18.9984
^{23}Na	22.9897726(16)	22.9898	22.9897707(20)	22.9898
^{27}Al	26.9815349(21)	26.9815	26.9815389(19)	26.9815
^{31}P	30.9737634(15)	30.9738	30.9737647(15)	30.9738
^{45}Sc	44.9559189(42)	44.956	44.9559189(33)	44.9559
^{55}Mn	54.9380536(41)	54.9380	54.9380503(35)	54.9380
^{59}Co	58.9331891(46)	58.9332	58.9331893(38)	58.9332
^{75}As	74.921580(50)	74.9216	74.9215964(39)	74.9216
^{89}Y	88.905430(90)	88.905	88.9058719(48)	88.9059
^{93}Nb	92.906020(110)	92.906	92.906382(5)	92.9064
^{103}Rh	102.90480(20)	102.905	102.9055110(48)	102.9055
^{127}I	126.904352(23)	126.9044	126.9044698(43)	126.9045
^{133}Cs	132.905090(150)	132.905	132.905355(38)	132.9055
^{141}Pr	140.907390(46)	140.907	140.907596(18)	140.9077
^{159}Tb	158.92430(110)	158.924	158.925351(26)	158.9254
^{165}Ho	164.93026(15)	164.930	164.930421(21)	164.9303
^{169}Tm	168.93434(15)	168.934	168.934245(34)	168.9342
^{197}Au	196.96666(10)	196.967	196.966541(10)	196.9665
^{209}Bi	208.980417(27)	208.980	208.980394(8)	208.9806
^{232}Th	232.038211(42)	232.038	232.038124(21)	232.0381
^{231}Pa	231.035936(42)	No entry	231.035877(22)	231.0359

Table II. Atomic Mass and Atomic Weight Values, 1971 - 1977

Nuclide	1971 At. Mass	1971 At. Weight	1977 At. Mass	1977 At. Weight
^{9}Be	9.0121828(6)	9.01218	9.0121825(4)	9.01218
^{19}F	18.9984046(7)	18.99840	18.99840325(14)	18.998403
^{23}Na	22.9897703(16)	22.98977	22.9897697(9)	22.98977
^{27}Al	26.9815406(9)	26.98154	26.9815413(7)	26.98154
^{31}P	30.9737633(9)	30.97376	30.9737634(7)	30.97376
^{45}Sc	44.9559174(22)	44.9559	44.9559136(15)	44.9559
^{55}Mn	54.9380464(27)	54.9380	54.9380463(17)	54.9380
^{59}Co	58.9331879(30)	58.9332	58.9331978(16)	58.9332
^{75}As	74.9216003(25)	74.9216	74.9215955(24)	74.9216
^{89}Y	88.9058667(32)	88.9059	88.9058560(32)	88.9059
^{93}Nb	92.9063803(32)	92.9064	92.9063780(31)	92.9064
^{103}Rh	102.905512(5)	102.9055	102.905503(5)	102.9055
^{127}I	126.9044755(36)	126.9045	126.904477(5)	126.9045
^{133}Cs	132.905436(8)	132.9054	132.905433(9)	132.9054
^{141}Pr	140.907698(11)	140.9077	140.907657(6)	140.9077
^{159}Tb	158.925386(12)	158.9254	158.925350(6)	158.9254
^{165}Ho	164.930357(11)	164.9304	164.930332(6)	164.9304
^{169}Tm	168.934245(11)	168.9342	168.934225(6)	168.9342
^{197}Au	196.966548(6)	196.9665	196.966560(6)	196.9665
^{209}Bi	208.980401(7)	208.9804	208.980388(5)	208.9804
^{232}Th	232.038074(11)	232.0381	232.0380538(25)	232.0381
^{231}Pa	231.035902(11)	231.0359	231.0358809(33)	231.0359

Table III. Atomic Mass and Atomic Weight Values, 1983 - 1995

Nuclide	1983 At. Mass	1985 At. Weight	1993 At. Mass	1995 At. Weight
^{9}Be	9.0121822(4)	9.012182(3)	9.0121822(4)	9.012182(3)
^{19}F	18.99840322(15)	18.9984032(9)	18.99840320(7)	18.9984032(5)
^{23}Na	22.9897677(10)	22.989768(6)	22.98976966(26)	22.989770(2)
^{27}Al	26.9815386(8)	26.981539(5)	26.98153841(24)	26.981538(2)
^{31}P	30.9737620(6)	30.973762(4)	30.97376149(27)	30.973761(2)
^{45}Sc	44.9559100(14)	44.955910(9)	44.9559102(12)	44.955910(8)
^{55}Mn	54.9380471(16)	54.93805(1)	54.9380493(15)	54.938049(9)
^{59}Co	58.9331976(16)	58.93320(1)	58.9331999(15)	58.933200(9)
^{75}As	74.9215942(17)	74.92159(2)	74.9215966(18)	74.92160(2)
^{89}Y	88.905849(3)	88.90585(2)	88.9058485(26)	88.90585(2)
^{93}Nb	92.9063772(27)	92.90638(2)	92.9063762(24)	92.90638(2)
^{103}Rh	102.905500(4)	102.90550(3)	102.905504(3)	102.90550(2)
^{127}I	126.904473(5)	126.90447(3)	126.904468(4)	126.90447(3)
^{133}Cs	132.905429(7)	132.90543(5)	132.905447(3)	132.90545(2)
^{141}Pr	140.907647(4)	140.90765(3)	140.907648(3)	140.90765(2)
^{159}Tb	158.925342(4)	158.92534(3)	158.925343(3)	158.92534(2)
^{165}Ho	164.930319(4)	164.93032(3)	164.930319(3)	164.93032(2)
^{169}Tm	168.934212(4)	168.93421(3)	168.934211(3)	168.93421(2)
^{197}Au	196.966543(4)	196.96654(3)	196.966551(3)	196.96655(2)
^{209}Bi	208.980374(5)	208.98037(3)	208.980384(3)	208.98038(2)
^{232}Th	232.0380508(23)	232.0381(1)	232.0380495(22)	232.0381(1)
^{231}Pa	231.035880(3)	231.03588(2)	231.0358780(28)	231.03588(2)