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ON THE ATOMIC MASSES (WEIGHTS?) OF THE ELEMENTS

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Abstract

Atomic masses (weights?) is an essential information for mining and metallurgy. The paper discusses four subjects around this problem. First, the classification of all the elements is suggested into 4 classes, based on their isotope features, determining the accuracy of their known atomic masses. As part of that, the class of elements is discussed with uncertain atomic weights in accordance with the 2009 IUPAC recommendations. A better (easier to use) format of atomic weights is presented for this class of elements. Third, it is found not informative to leave empty spaces instead of approximate atomic weights for elements with unstable isotopes. Fourth, the term atomic weight vs the term atomic mass is discussed shortly, in agreement with the SI system of units and in contrary to the questionable IUPAC convection.

Key words: Atomic mass; IUPAC, Atomic weight; Isotopes.

1. Introduction

In metallurgical laboratories and plants the weight (mass, m, kg) of chemical substances are measured for experiments and production. In classrooms, technical reports and scientific papers the phenomena taking place during the experiments or production are discussed in terms of amount of material (n, mole). The connection between them is expressed using atomic masses (M, kg/mol), through the well known equation:

$$m = M \cdot n \qquad (1)$$

Eq.(1) makes the atomic masses of the elements their most important basic property.

Atomic weights are relative values, expressed relative to the exact (by definition) mass of 0.012 kg of 1 mole of isotope C-12 (see the discussion of “mole” [1]). There is a

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natural desire of all of us to know the atomic masses of all elements with as high accuracy as possible. At this point it is important to note that due to their relative nature, atomic weights are not limited even by the relative standard uncertainty (5 10^{-8}) of the Planck constant [1-2], giving a natural limit for the definition of kilogram (although today it is still defined through an international artifact [1, 3]). Atomic weights are determined by the following general equation:

$$M = \sum_i x_i \cdot M_i \quad (2)$$

with x_i – the mole fraction of isotope i of the given element, M_i is the relative atomic mass of the isotope i of the given element. The atomic mass of the isotopes is mainly measured in physical laboratories, while isotope fractions are measured by chemists.

IUPAC publishes biennial reviews on “best” atomic weights of the elements. In previous years the 2007 standard data were used [4]. Recently, the 2009 standard data have been published [5], accompanied by a more popular presentation [6], including also a tear-off page of the most recent periodic table of IUPAC with the most recent “best” atomic weights. It is envisioned that this periodic table will be the basis of our education and practice in the near future.

This paper is written to discuss and improve the format of some values given in this standard IUPAC table, without arguing the validity of the values themselves. Also, a 4-level division is suggested here for the 112 elements based on the accuracy of the atomic weights and the reasons behind.

2. On the four classes of elements based on the features of their isotopes

The four classes of elements will be presented here in order of the decreasing accuracy of their atomic weights (see Table 1). The basis for classification is the special features of the isotopes of different elements.

2.1. Class A

In class A there are 22 elements: Be, F, Na, Al, P, Sc, Mn, Co, As, Y, Nb, Rh, I, Cs, Pr, Tb, Ho, Tm, Au, Bi, Th, Pa. The main characteristic feature of this class of elements is that they have only one known isotope, with its mole fraction of 1 [7]. That is why the atomic weights of these elements have the highest accuracy, not limited by the accuracy of x_i measurements. Atomic weights of these elements are known by 7 – 10 digits of accuracy and can be considered as constants of nature.

The number of elements in this class is not expected to increase. In the contrary, it

Table 1. Classification of elements according to the features of their isotopes

Class	Members	Characteristic feature	Format of M	Accurate digits in M
A	22	Only one isotope	22.98976928(2)	7 … 10
B	52	No variable isotope composition	112.411(8)	4 … 8
C	10	Variable isotope composition	$32.065(5)^{+0.011}_{-0.006}$	3 … 5
D	28	No stable isotope	(145)	3

might decrease in future, if a second isotope of any of the elements is discovered.

2.2 Class B

In class B there are 52 elements: He, Ne, Mg, Ar, K, Ca, Ti, V, Cr, Fe, Ni, Cu, Zn, Ga, Ge, Se, Br, Kr, Rb, Sr, Zr, Mo, Ru, Pd, Ag, Cd, In, Sn, Sb, Te, Xe, Ba, La, Ce, Nd, Sm, Eu, Gd, Dy, Er, Yb, Lu, Hf, Ta, W, Re, Os, Ir, Pt, Hg, Pb, U. The main characteristic feature of this class of elements is that although they have more than one isotope [7], but the mole fraction of those isotopes was not found to vary in different terrestrial samples beyond the accuracy of the measurements [5]. Thus, the accuracy of the atomic weight depends on the accuracies of measured x_i and M_i values. That is why the atomic weights of these elements are known by a less accuracy compared to class A (see Table 1). The atomic weights of these elements can also be considered as constants of nature, at least for natural terrestrial samples.

The number of elements in this class is expected to decrease in the future, as some of the elements are expected to migrate to class C as the accuracy to measure isotope compositions improves further, or if a larger variety of terrestrial samples are carefully analyzed. On the other hand, some elements might migrate into this class from class A, if new isotopes of some of those elements are discovered in the future.

2.3. Class C

In class C there are 10 elements: H, Li, B, C, N, O, Si, S, Cl, Tl. The main feature of this class of elements is that they have more than one isotope [7], and the mole fractions of those isotopes were found to vary in different terrestrial samples beyond the accuracy of the measurements [5].

This fact was first recognized by IUPAC in its 2011-publication of the 2009 atomic weights [5-6]. It is a very important step in understanding nature. It means that the atomic weights of these elements are not constants of nature any more, but depend upon the physical, chemical, and nuclear history of the sample material. Instead of a given value for the standard atomic weight [4], IUPAC now suggests to use an interval of values for the standard atomic weight. For example, for Li the 2007 standard atomic weight was: M_{Li} = 6.941(2) g/mol, while the 2009 standard atomic weight is: M_{Li} = [6.938; 6.997] g/mol. It is important to understand that the average value of this interval (6.968 g/mol) does not represent the most probable value in an average natural terrestrial sample (6.941(2) g/mol). The meaning of the given interval is that all natural terrestrial samples fall into this interval (to our best knowledge). This interval is dictated not by the accuracy of measurements, rather by nature.

The present author welcomes this major step of IUPAC to express the reality of nature in it’s new table of atomic weights. However, the present author does not agree with the format suggested by IUPAC. If only the information M_{Li} = [6.938; 6.997] g/mol is given to the users, an average user will inevitably use the average value (6.968 g/mol) for practical calculations, even if IUPAC clearly states that it should not be done [5-6]. By doing so, the average user will make an error in the 3rd digit compared to the average terrestrial sample. It should be noted at this point that Table 6 of the original IUPAC review [5] provides “Conventional atomic weights 2009 for users needing an atomic weight value for an unspecified sample”. However, in the accompanying publication and in its tear-off periodic table this information is lost [6]. Moreover, the table of conventional atomic weights [5] loses the very important finding of IUPAC on the variable nature of natural terrestrial samples.

Therefore, herewith the following format to present the atomic weights of this class of elements is suggested (for Li, as an example): $M_{Li} = 6.941(2)^{+0.056}_{-0.003}$ g/mol. Here, the “best” average value is taken from the 2007 IUPAC value, while the ± ranges are defined in a way to satisfy the 2009 IUPAC values[1]. The following explanations should accompany atomic weights given in the format of $M_{Li} = 6.941(2)^{+0.056}_{-0.003}$ g/mol:

i. in general calculations (carried out for unspecified samples) the value of 6.941(2) g/mol should be used for Li;

ii. for elements with this format the atomic weights were found to vary from sample to sample beyond the accuracy of measurements;

iii. possible interval of atomic weights for Li is calculated as 6.941 – 0.003 = 6.938 g/mol (minimum possible value) and 6.941 + 0.056 = 6.997 g/mol (maximum possible value), giving the following interval of atomic weights of Li in terrestrial samples: [6.938; 6.997] g/mol.

The number of elements in class C is expected to increase by some further elements to be transferred here from class B, with the increase of accuracy of measurements, or if a larger variety of terrestrial samples is carefully examined.

2.4. Class D

In class D there are 28 elements: Tc, Pm, Po, At, Rn, Fr, Ra, Ac, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn. The characteristic feature of these elements is that they do not have stable isotopes [7], and thus they cannot be provided by an atomic weight value characterizing an average natural terrestrial sample. That is why IUPAC provides no information at all on the atomic weights of these elements [4-6]. Although the scientific reasons of this decision are well understood, it is not practical from the point of view of understanding chemistry and natural sciences. If we follow this practice and disseminate periodic tables with empty spaces for the atomic weights of class D elements, more and more people will incorrectly suppose that we have no idea what the atomic weight of these elements might be. This is certainly not the case. In fact, partly stable isotopes are known for each of these elements with their measured isotopic masses and half-lives [5]. The higher is the half life of an isotope, the longer it exists, thus the higher is its molar ratio within the isotopes of the given element. Thus, Eq.(2) can be modified to estimate the average atomic weight of this class of elements through the half lives of the isotopes:

$$M \cong \frac{\sum_i \tau_i \cdot M_i}{\sum_i \tau_i} \tag{3}$$

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[1] If this format is accepted, the best average value can be improved by IUPAC at a later date.

with τ_i – half life (s) of isotope i of the given element with a relative isotope mass of M_i. The average atomic weights calculated by Eq.(3) are suggested to be included in the table of standard atomic weights, rounded to 3 digits and presented in parenthesis. The parenthesis means that the element is not found in natural terrestrial samples. However, the approximated value up-to 3 digits of accuracy provides reasonably accurate information compared to the empty space provided today in standard IUPAC tables. For example, for element 112 the following value is found by Eq.(3): M_{Cn} = (285) g/mol.

To check the estimating ability of Eq.(3) three A-B class elements (Th, Pa, U) are used with known isotope composition [7], but with the given half-lives [5]. It is found that the values calculated from Eq.(3) and rounded to 3 digits using data of [5], coincide with independent standard values calculated from measured isotope mole fractions [7] and also rounded to 3 digits (see [5]). This confirms the validity of Eq.(3).

The number of elements in class D is expected to increase in time, as IUPAC will recognize more and more elements beyond the present threshold of 112 (most probably all elements with atomic numbers higher than 112 have no stable isotopes).

In Table 2 the "best" atomic weights of all 112 elements are given. The classes A-B-C-D defined above are given for each element. For classes A-B the data of [5] are given. For classes C-D the above formats are used and the data given in [4-5] are combined with Eq.(3) to find the appropriate values.

Table 2. The atomic weight of elements in a new, suggested format

Atomic number	Symbol	Class	Atomic weight, g/mol
1	H	C	$1.00794(7)^{+0.00017}_{-0.00010}$
2	He	B	4.002602(2)
3	Li	C	$6.941(2)^{+0.056}_{-0.003}$
4	Be	A	9.012182(3)
5	B	C	$10.811(7)^{+0.010}_{-0.005}$
6	C	C	$12.0107(8)^{+0.0009}_{-0.0011}$
7	N	C	$14.0067(2)^{+0.00058}_{-0.00027}$
8	O	C	$15.9994(3)^{+0.00037}_{-0.00037}$
9	F	A	18.9984032(5)
10	Ne	B	20.1797(6)
11	Na	A	22.98976928(2)
12	Mg	B	24.3050(6)
13	Al	A	26.9815386(8)
14	Si	C	$28.0855(3)^{+0.0005}_{-0.0015}$
15	P	A	30.973762(2)
16	S	C	$32.065(5)^{+0.011}_{-0.006}$
17	Cl	C	$35.453(2)^{+0.004}_{-0.007}$
18	Ar	B	39.948(1)
19	K	B	39.0983(1)
20	Ca	B	40.078(4)
21	Sc	A	44.955912(6)
22	Ti	B	47.867(1)
23	V	B	50.9415(1)
24	Cr	B	51.9961(6)
25	Mn	A	54.938045(5)
26	Fe	B	55.845(2)
27	Co	A	58.933195(5)
28	Ni	B	58.6934(4)
29	Cu	B	63.546(3)
30	Zn	B	65.38(2)
31	Ga	B	69.723(1)
32	Ge	B	72.63(1)
33	As	A	74.92160(2)
34	Se	B	78.96(3)
35	Br	B	79.904(1)
36	Kr	B	83.798(2)

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37	Rb	B	85.4678(3)
38	Sr	B	87.62(1)
39	Y	A	88.90585(2)
40	Zr	B	91.224(2)
41	Nb	A	92.90638(2)
42	Mo	B	95.96(2)
43	Tc	D	(97.5)
44	Ru	B	101.07(2)
45	Rh	A	102.90550(2)
46	Pd	B	106.42(1)
47	Ag	B	107.8682(2)
48	Cd	B	112.411(8)
49	In	B	114.818(3)
50	Sn	B	118.710(7)
51	Sb	B	121.760(1)
52	Te	B	127.60(3)
53	I	A	126.90447(3)
54	Xe	B	131.293(6)
55	Cs	A	132.9054519(2)
56	Ba	B	137.327(7)
57	La	B	138.90547(7)
58	Ce	B	140.116(1)
59	Pr	A	140.90765(2)
60	Nd	B	144.242(3)
61	Pm	D	(145)
62	Sm	B	150.36(2)
63	Eu	B	151.964(1)
64	Gd	B	157.25(3)
65	Tb	A	158.92535(2)
66	Dy	B	162.500(1)
67	Ho	A	164.93032(2)
68	Er	B	167.259(3)
69	Tm	A	168.93421(2)
70	Yb	B	173.054(5)
71	Lu	B	174.9668(1)
72	Hf	B	178.49(2)
73	Ta	B	180.94788(2)
74	W	B	183.84(1)
75	Re	B	186.207(1)
76	Os	B	190.23(3)
77	Ir	B	192.217(3)
78	Pt	B	195.084(9)
79	Au	A	196.966569(4)
80	Hg	B	200.59(2)
81	Tl	C	$214.3833(2)^{+0.0017}_{-0.0013}$
82	Pb	B	207.2(1)
83	Bi	A	208.98040(1)
84	Po	D	(209)
85	At	D	(210)
86	Rn	D	(220)
87	Fr	D	(219)
88	Ra	D	(226)
89	Ac	D	(227)
90	Th	A	232.03806(2)
91	Pa	A	231.03588(2)
92	U	B	238.02891(3)
93	Np	D	(237)
94	Pu	D	(244)
95	Am	D	(243)
96	Cm	D	(247)
97	Bk	D	(247)
98	Cf	D	(251)
99	Es	D	(253)
100	Fm	D	(257)
101	Md	D	(259)
102	No	D	(259)
103	Lr	D	(256)
104	Rf	D	(265)
105	Db	D	(268)
106	Sg	D	(270)
107	Bh	D	(269)
108	Hs	D	(277)
109	Mt	D	(276)
110	Ds	D	(281)
111	Rg	D	(280)
112	Cn	D	(285)

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3. Atomic weights against atomic masses

According to the SI system of units [3], the unit of mass is kg (or g), therefore the molar atomic mass has a unit of g/mol. On the other hand, weight is dependent on the acceleration due to gravity, which is an ill-defined quantity even along the surface of the Earth.

Therefore, atomic masses rather than atomic weights should be used in all scientific writing. In this paper atomic weights have been sometimes used to be in agreement with the present IUPAC wording [4-6]. However, it is suggested here that this wording should be changed and published by IUPAC, in accordance with the SI system.

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References

[1] G. Kaptay, On the five base quantities of nature and SI (The International System of Units), J. Min. Metall. Sect. B-Metall. 47 (2) B (2011) 241-246.

[2] P.J. Mohr, B.N. Taylor, D.B. Newell: CODATA recommended values of the fundamental physical constants: 2006. Rev. Modern Phys., (80) (2008) 633-730.

[3] The International System of Units (SI), 8th edition, 2006. http://www.bipm.org/utils/common/pdf/si_brochure_8_en.pdf

[4] M.E. Wieser, M. Berglund: Atomic weights of the elements 2007 – Pure Appl. Chem., 81(11) (200) 92131-2156.

[5] M.E. Wieser, T.B. Coplen: Atomic weights of the elements 2009 – Pure Appl. Chem., 83 (2) (2011) 359-396.

[6] T.B. Coplen, N.E. Holden: Atomic Weights – no longer constants of nature – Chem. Int., 2011, March-April, 10-15.

[7] M. Berglund, M.E. Wieser: Isotopic compositions of the elements 2009 – Pure Appl. Chem., 83 (2) (2011) 397-410.