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Atomic Weights Change and the Mole is Redefined

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Abstract: The chemistry community is encouraged to keep up to date with revisions to standard atomic weights and definitions of SI base units, including the mole.

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Over the last 60 years, I have either been a pupil or teacher in a classroom, laboratory, or lecture hall with a periodic table hanging on the wall. The periodic table displayed was typically never renewed during my residence in a given teaching area. This is both disappointing and a failure of the education system. Most obviously, the number of elements has grown over the years and currently stands at 118.^[1,2] Secondly, the International Union of Pure and Applied Chemistry (IUPAC) regularly revises atomic weights based on new determinations of the isotopic abundances of the elements on Earth. An overview of the most recent updates is given in an IUPAC Technical Report published in 2021,^[3] and salient points from this report with background information are summarised in this Chemical Education Column along with the 2019 revised definition of the mole.

Standard Atomic Weights

The *standard atomic weight of an element*, A_r° , is defined by IUPAC as the “*recommended value of atomic weight (relative atomic mass) of an element revised biennially by the Commission on Isotopic Abundances and Atomic Weights (CIAAW) and applicable to elements in any normal material with a high level of confidence*”.^[3] A normal material excludes those with artificial isotopic changes, extraterrestrial materials, or isotopically anomalous materials (*e.g.* products from a nuclear reactor). The value of A_r° is stated either as a value with an uncertainty (used for 71 elements) or as an interval (used for 14 elements). To understand this difference, we need to step back to the first half of the 20th Century when it was first recognised that the atomic weight of certain elements, such as Pb and S, varied depending on the natural source from which the element was obtained. In 1969, uncertainties were included in all atomic weights to account, not only for measurement errors but also, more importantly, for the natural variation in isotopic compositions.^[4] Of the 118 elements in the modern periodic table, 21 (*e.g.* Be, F, P, Au) possess one stable isotope and A_r° for each element is a constant value, known extremely accurately. For example, A_r° for F = 18.998 403 162 ± 0.000 000 005 or 18.998 403 162(5). The uncertainty in A_r° may be small or large for elements with two or more isotopes. For example, for silver with isotopes ¹⁰⁷Ag and ¹⁰⁹Ag, $A_r^\circ = 107.8682(2)$, while for ruthenium with isotopes ⁹⁶Ru, ⁹⁸Ru, ⁹⁹Ru, ¹⁰⁰Ru, ¹⁰¹Ru, ¹⁰²Ru, ¹⁰⁴Ru, $A_r^\circ = 101.07(2)$.

By the mid-1900s, it was already recognised that elements such as H, B, C, O, Si, and S exhibited variations in the abundances of their stable isotopes depending upon the source of the material. This leads to a range of atomic weights for a given element. One solution adopted by the IUPAC was to consider the range of A_r values, determine the median value as A_r° , and calculate an uncertainty based on these data. Periodic tables that many readers still use routinely will give a value of A_r° for H as 1.007 94(7). In 2009, a change to the use of *intervals* was introduced to better account for the variation in atomic weight values in natural terrestrial materials.^[5] The decision by IUPAC to assign A_r° either as a value with an uncertainty or as an interval is made on an element-by-element basis for various reasons.^[5] The value of A_r° for H is now expressed as [1.007 84, 1.008 11] rather than 1.007 94(7). This means that the atomic weight of any terrestrial sample of hydrogen will lie between 1.007 84 and 1.008 11. The interval notation is currently used for 14 elements: H, Li, B, Br, C, N, O, Mg, Si, S, Cl, Ar, Tl, and Pb. Thus, for Pb, the standard atomic weight is now given as [206.14, 207.94] rather than 207.2 ± 0.1 or 207.2(1), the change to an interval being made in 2021. Of course, using intervals causes some difficulty when one needs a value of atomic weight for a calculation, *e.g.* determining the number of moles of a compound. In this case, IUPAC also defines a conventional A_r value, *e.g.* 1.008 for H (Fig. 1), and 207.2 for Pb.^[3] Where an interval for an element is defined by the IUPAC, use of the single value of A_r in calculations can only give an approximate answer.

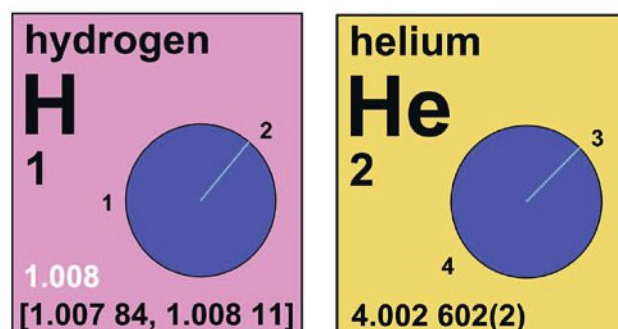


Fig. 1. Cells from the IUPAC Periodic Table of the Elements and Isotopes (IPTeI) for H and He. The pie-charts show the stable isotope abundances (¹H, ²H, and ³He, ⁴He). A background colour of pink signifies that an element has two or more isotopes which are used to determine its atomic weight and the variation in isotopic abundances and atomic weights in normal materials is large and well known; A_r° is given as lower and upper limiting values, written in square brackets []. For laboratory calculations, commerce and industry, a conventional A_r value is shown in white (1.008 for H). A background colour of yellow signifies that an element has two or more isotopes used to determine its atomic weight. A_r° is defined as a single value with an uncertainty. (Reproduced with permission from “IUPAC Periodic Table of the Elements and Isotopes (IPTeI) for the Education Community”, *Pure Appl. Chem.* **2018**, 90, 1833).

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The IUPAC Periodic Table of the Elements and Isotopes (IPTEI) has been specifically designed for educational purposes.^[6] Each element cell in the IPTEI displays isotopic abundances as a pie-chart, and the background colour of element's cell is coded to indicate whether one (*e.g.* P, As) or more (*e.g.* H and He, Fig. 1) isotopes are used to determine the atomic weight of the element, whether the standard atomic weight is given as a single value with an uncertainty (*e.g.* He, K, Ti), whether the standard atomic weight is given as lower and upper limits (*e.g.* H, Mg, Pb), or whether all the element's isotopes are radioactive and no isotope occurs in normal materials with a characteristic terrestrial isotopic composition (*e.g.* Tc). There can be no standard atomic weight for an element with no stable isotopes; only the atomic mass of each isotope can be specified (*e.g.* Tc, two radioactive isotopes with atomic masses of 96.90636 and 97.90721, respectively). The report^[6] that introduces the IPTEI also provides a detailed summary of applications of isotopes in biology, medicine, forensic science, geochronology, Earth and planetary science and industry, and illustrates sources of radioisotopes.

Revised Definition of the Mole

The mole is one of the seven base units in the SI system (Système International d'Unités): the metre, kilogram, second, ampere, kelvin, candela, and mole. Between 1971 and 2019, the mole was defined “*as the amount of a substance containing as many elementary entities as there are atoms in 0.012 kilogram of carbon-12*”, and one mole of a substance (atoms, ions, molecules, electrons, or other entities) contained the Avogadro number of particles.

In 2018, the General Conference on Weights and Measures^[7] approved revised definitions of the kilogram, mole, ampere, and kelvin, based on fundamental constants (Planck constant, Avogadro constant, elementary charge, and Boltzmann constant). Part of the reasoning behind the revision was that “*SI units must be stable in the long term, internally self consistent and practically realizable being based on the present theoretical description of nature at the highest level*”.^[7] Before 2019, the kilogram was defined as the mass of a platinum-iridium cylinder retained at the International Bureau of Weights and Measures in Paris. An international collaboration called the Avogadro Project was set up to measure the Avogadro constant very precisely and thus enable the kilogram to be defined with respect to this physical constant. The number $6.022\,140\,76 \times 10^{23}$ is now defined as the *exact* value of the Avogadro constant and the definition of the mole was revised in 2019, with the mole being redefined in terms of the Avogadro constant:^[3,8]

One mole of a substance contains exactly $6.022\,140\,76 \times 10^{23}$ elementary entities.

The change in definition results in the mass of a mole of carbon-12 atoms no longer being exactly 0.012 kg. The change in the definition has no impact on chemists' practical activities, and only affects the calculation of molar masses to very high precisions.

Closing remarks

It is all too easy to think that definitions are set in stone. In this column, I have emphasised that the CIAAW reassesses atomic weights every two years. Thus, the *IUPAC Periodic Table of the Elements and Isotopes* published in 2018 shows A_r° for Pb = 207.2(1), but in 2021, this was updated to an interval of [206.14, 207.94]. It is difficult to keep up, but as more accurate isotopic abundance measurements are published, standard atomic weights are bound to change. It is important that the educators of future

generation scientists attempt to follow the updates, to keep their cohorts of students aware of the ever-changing scientific horizon.

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- [1] P.J. Karol, R.C. Barber, B.M. Sherrill, E. Vardaci, T. Yamazaki, *Pure Appl. Chem.* **2016**, *88*, 115. <https://doi.org/10.1515/pac-2015-0501>
- [2] L. Öhrström, J. Reedijk, *Pure Appl. Chem.* **2016**, *88*, 1225. <https://doi.org/10.1515/pac-2016-0501>
- [3] T. Prohaska, J. Irrgeher, J. Benefield, J.K. Böhlke, L.A. Chesson, T.B. Coplen, T. Ding, P.J.H. Dunn, M. Gröning, N.E. Holden, H.A.J. Meijer, H. Moossen, A. Possolo, Y. Takahashi, J. Vogl, T. Walczyk, J. Wang, M.E. Wieser, S. Yoneda, X.-K. Zhu, J. Meija, *Pure Appl. Chem.* **2021**, *94*, 573. <https://doi.org/10.1515/pac-2019-0603>
- [4] T.B. Coplen, N.E. Holden, *Chem. Int.* **2011**, *33*, 10. <https://doi.org/10.1515/ci.2011.33.2.10>
- [5] M.E. Wieser, T.B. Coplen, *Pure Appl. Chem.* **2011**, *83*, 359. <https://doi.org/10.1351/PAC-REP-10-09-14>
- [6] N.E. Holden, T.B. Coplen, J.K. Böhlke, L.V. Tarbox, J. Benefield, J.R. de Laeter, P.G. Mahaffy, G. O'Connor, E. Roth, D.H. Tepper, T. Walczyk, M.E. Wieser, S. Yoneda, *Pure Appl. Chem.* **2018**, *90*, 1833. <https://doi.org/10.1515/pac-2015-0703>
- [7] <https://www.bipm.org/en/committees/cg/cgpm/26-2018/resolution-1> (accessed 30 May 2024).
- [8] <https://www.nist.gov/si-redefinition/redefining-mole> (accessed 30 May 2024).