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Goodbye to the Non-SI unit dalton (Da) in the Digital-SI?

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Summary:
The need to develop an unambiguous digital version of the International System of units (SI) leads to a reconsideration of the status of the Non-SI units accepted for use with the SI. Here is considered the case of the Non-SI unit dalton that coexists with the kilogram in the field of atomic masses.

Keywords: metrology, kilogram, dalton (Da), digital SI, atom interferometry.

Atomic masses in Si and Non-SI units

The redefinition of the SI, the International System of units, ended with decades coexisting two systems of electrical units by fixing the values of the Planck constant h and the elementary charge e in the definitions of the kilogram and the ampere respectively. But we continue to live with two units of mass. For historical and technical reasons, the dalton is still used in atomic mass measurements instead of the kilogram. The dalton (Da) and the unified atomic mass unit (m_u) are alternative names for the same unit, equal to 1/12 of the mass of a free carbon 12 atom, at rest and in its ground state. The consequences of revising the SI for measurements in chemistry were analyzed in advance by IUPAC, the International Union of Pure and Applied Chemistry. A IUPAC technical report published in 2017 [1] stated that, since the masses of the nuclides are reported in the unified atomic mass unit, in the case of fixing the values of the Planck constant h and the Avogadro number N_A, as really occurred, the Atomic Mass Evaluations published at regular intervals by IUPAC would remain unaffected.

The kilogram is reaching the Dalton (Da)

The redefinition of the SI opened up improvements and new possibilities across the whole mass scale, especially in the range of atomic masses. Being the kilogram defined in terms of the Planck constant, the realization of mass can be achieved at any desired scale without the need to trace the measurements to a 1 kg mass. Employing atom interferometry, the measurement of the recoil velocity of an atom of mass m that absorbs a photon of momentum $\hbar k$, yields the ratio h/m ($\hbar = h/2\pi$ and $k = 2\pi/\lambda$, where λ is a laser wavelength). Because the value of the Planck constant h has been fixed in the new SI, the ratio h/m_u ensures the realization of the kilogram at the atomic scale. Furthermore, as the Avogadro constant has been also fixed, and the carbon molar mass $M(^{12}C)$ is no longer equal to 12g per mol, it is now determined from m_u. Before the redefinition of the SI the accuracy of atomic masses expressed in kg was in the order of 10^{-8}, well above the minor uncertainties reached in terms of the dalton. The last value recommended by CODATA at that time for the equivalence between kg and dalton was 1 Da = 1.660 539 040 × 10^{-27} kg, with a relative standard uncertainty of 1.2×10^{-8}. From the value of the ratio h/m_u, the uncertainty in the ratio dalton to kilogram just after fixing h was reduced in more than one order of magnitude.

Tab. 1: Evolution of the relative standard uncertainties of $h/m(^{133}Cs)$ and $h/m(^{88}Rb)$

Source	$h/m(^{133}Cs)$	$h/m(^{88}Rb)$	h/m_u
CODATA 2002	1.5×10^{-8}		6.7×10^{-9}
CODATA 2006	1.5×10^{-8}	1.3×10^{-8}	1.4×10^{-9}
CODATA 2010	1.5×10^{-8}	1.2×10^{-9}	7.0×10^{-10}
CODATA 2014	1.5×10^{-8}	1.2×10^{-9}	4.5×10^{-10}
Berkeley 2018	4.0×10^{-10}		
Paris 2020		$\mathbf{1.4\times10^{-10}}$	

The new SI is effective from 20 May 2019. Short after that date, some considerations on the future of the SI were already published [2], including last data showing how h/m(X) measurements using atom interferometry were evolving from 2002, as recorded by CODATA. X may be ^{87}Rb atoms, as determined at the Laboratoire Kastler Brossel LKB in Paris, or ^{133}Cs atoms, as determined in the University of California in Berkeley. The 2022 CODATA adjustment of the fundamental constants is the next regularly scheduled adjustment, with a closing date of 31 December. Table 1 shows the evolution of *h/m* values, including now the last value obtained at LKB in Paris in December 2020 [3]. This value for $m(^{87}\mathrm{Rb})$ is the most accurate atomic mass measurement, reducing the uncertainty in the equivalence between kg and dalton to the 10^{-10} level.

Towards a digital system of units

Building confidence in the accuracy and global comparability of measurements requires the creation of a machine-actionable, unambiguous full digital representation of the SI. There are ontologies and unified codes including all units of measurement used in science, engineering, and business (e.g. QUDT, UCUM). Here we adress an existing Guide for the use of the metadata-format used in metrology for communication between machines using only SI-base units [4]. The document was developed within the framework of the EU-funded project SmartCom, ended in September 2021, with the support of international partners from science and industry. Several major National Metrology Institutes participated (PTB, NPL, etc.). Only non-SI units accepted for use with the SI stated in the SI Brochure [5] may be included, but only during a transition period. Metrological data are categorized into 5 quality classes of machine readability: platinum, gold “2030”, silver “2024”, bronze “2020” and “improvable”. Platinum corresponds to the strongest readability. The SI unit kilogram is classified platinum and the Non-SI unit dalton is classified silver, recommending the use of the kg. A significant highlight is the creation within the International Committee for Weights and Measures (CIPM) of a Task Group on the Digital-SI. The aim is to consider, develop and establish a world-wide uniform, unambiguous and secure data exchange format for use in IoT networks based on the SI described in the current SI Brochure.

Discussion

The coexistence of SI units with Non-SI units introduces ambiguities. The joint use for some of them has been admitted in the SI Brochure without any time limit. The new paradigm of the digital transformation now requires making decisions that were not on the agenda of different communities using Non-SI units. In the 2017 critical review the IUPAC report [1] showed no interest in expressing atomic masses in the SI unit kilogram. The removal of the Non-SI unit dalton opening the way to the use of the kilogram on the atomic mass scale would not have such a high negative impact as before the redefinition of the SI, since the experimental uncertainties achieved in the most precise cases are very close. In table 1 we observe how close is the relative standard uncertainty of the m_u value from that of the values of the atomic masses used in atom interferometry experiments, particularly from the mass of ^{88}Rb. Holger Müller’s group in Berkeley is also working on improvements, intending to produce new $h/m(^{133}\mathrm{Cs})$ results with uncertainties below 10^{-10} in the near future. The most precisely atomic and ion relative masses are known at the 10^{-11} level [6].

The transition period stated in the Guide D-SI [4] for quality class silver, also called 2024, should be reviewed in order to obtain wider consensus from other communities that use Non-SI units accepted for use with the SI. For example, the replacement by the unit 1 of the Non-SI units neper, bel and decibel, as identified in Table A.4 of the Guide D-SI, would not be as easy to adopt as the replacement of the dalton by the kg. That topic exceeds this short paper and deserves to be addressed in a more extensive one. Finally, the eventual decision to delete some Non-SI units in the SI Brochure will also require some time until a new version is published

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