The New International System of Units: The Role of the Committee on Data for Science and Technology (CODATA)

D. B. Newell, P. J. Mohr, and B. N. Taylor

Abstract: *The mission of the Committee on Data for Science and Technology (CODATA) of the International Council for Science is to strengthen international science for the benefit of society by promoting improved scientific and technical data management and use. One of their most visible outputs comes from the Task Group on Fundamental Constants (TGFC), which periodically performs a comprehensive least-squares adjustment of the values of the constants and produces the well-known and widely cited publication entitled "CODATA recommended values of the fundamental physical constants: year" (freely available at http://physics.nist.gov/cuu/constants). When the proposal to change the International System of Units (SI) by redefining the kilogram, ampere, kelvin, and mole in terms of fixed values of the Planck constant h, elementary charge e, Boltzmann constant k, and Avogadro constant* N_A*, respectively, is implemented in the near future, it will be the responsibility of the TGFC to provide these values. In this presentation, the least-squares adjustment procedure will be outlined and illustrated with reference to current state-of-the-art measurements in several physical disciplines.*

1. Introduction

The International System of Units (SI) is the world-wide system of measurement for science, trade, and commerce. The origin of the SI can be traced back to the 1875 Convention of the Meter with the foundation of the measurement system being artifact standards. Since then the SI has been modified to incorporate new knowledge and better standards that are linked to fundamental constants and other invariants of nature, such as the 1983 redefinition of the meter based on an exact value of the speed of light in vacuum, $c = 299\ 792\ 458$ m/s. Today the SI is poised to be fully defined in terms of exact values of fundamental constants and properties of atoms as outlined in the International Committee for Weights and Measures (CIPM) Draft Resolution A for the 24[th] meeting of the General Conference on Weights and Measures (CGPM) [1]. Draft Resolution A proposes to redefine the kilogram, ampere, kelvin, and mole in terms of fixed values of the Planck constant h, elementary charge e, Boltzmann constant k, and Avogadro constant N_A, respectively. Resolution A also invites the Committee on Data for Science and Technology (CODATA) Task Group on Fundamental Constants (TGFC) to provide the adjusted values and uncertainties of the fundamental physical constants that will be used for the revised SI.

2. Formation of the CODATA Task Group on Fundamental Constants

The determination of the best or most probable values of the fundamental physical constants has traditionally been done by the method of least squares [2 to 5] as pioneered by Birge [6]. Subsequent determinations and adjustments were performed by various groups [7 to 16] inevitably leading to different recommended values of the fundamental constants, due in part to the use of different data and in part to different evaluation methods, especially when it came to treating discrepant data. In 1966 the International Council of Science (then the International Council of Scientific Unions) [17] established

CODATA [18] with the mission to strengthen international science for the benefit of society by promoting improved scientific and technical data management and use. Soon after, in 1969, CODATA established the TGFC [19] with the mission to periodically provide the scientific and technological communities with a self-consistent set of internationally recommended values of the basic constants and conversion factors of physics and chemistry based on all of the relevant data available at a given point in time.

The first official CODATA adjustment was performed in 1973 [20] with subsequent adjustments performed in 1986 [21], 1998 [22], 2002 [23], and 2006 [24]. The 2010 adjustment has recently been completed with the updated recommended values of the fundamental constants posted at http://physics.nist.gov/cuu/constants. The next routine CODATA adjustment in the current four-year cycle will be performed in 2014, unless the TGFC is requested by the CIPM before then to provide exact values of h, e, k, and N_A to establish the new SI.

3. The Role of the CODATA Task Group on Fundamental Constants

The motivation for and the philosophy behind the periodic adjustment of the values of the constants, and descriptions of how units, quantity symbols, numerical values, numerical calculations, and uncertainties are treated, in addition to how the data are characterized, selected, and evaluated, can be found in detail in the 1998, 2002, and 2006 adjustment reports [22, 23, 24]. It is important to highlight the key differences between the methodology of the TGFC and other data analyses.

First, the underlying philosophy has been to provide the user community with values of the constants having the smallest possible uncertainties consistent with the information available at the time. The motivation for this approach is that it gives the most critical users of the values of the constants the best possible tools for their work based on the current state of knowledge. The downside is that the information available may include an error or oversight. Nevertheless, the CODATA TGFC rejects the idea of making uncertainties sufficiently large that any future change in the recommended value of a constant will likely be less than its uncertainty. The Task Group does not employ 'safety factors' such as maximal consistent subsets, outlier exclusion, guard-banding, uncertainty lower-limit cutoffs, and unknown bias estimation,

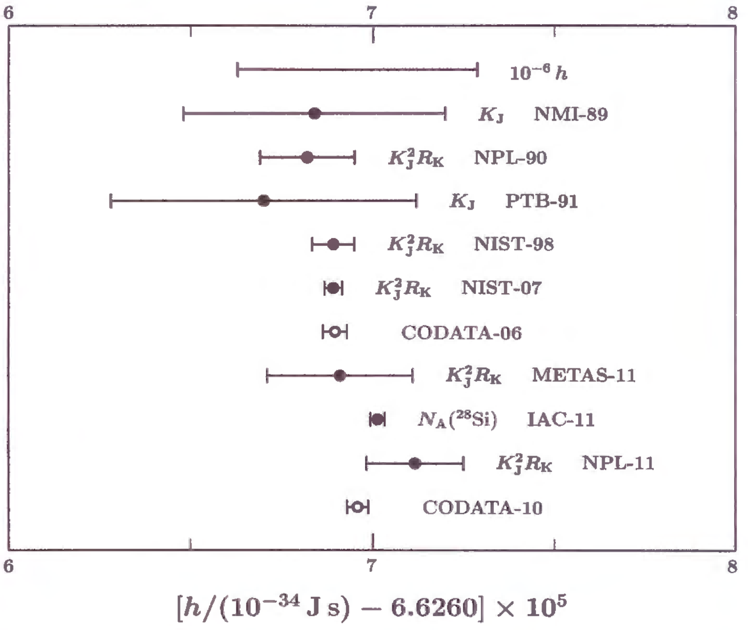

Figure 1. Input data related to the 2010 CODATA TGFC determination of the Planck constant. Data are from a Hg electrometer, NML-89; a capacitor voltage balance, PTB-91; five watt balances, NPL-90, NIST-98, NIST-07, METAS-11, NPL-11; and the International Avogadro Coordination project's determination of N_A using the x-ray-crystal-density (XRCD) method, IAC-11. In the figure, $K_J = 2e/h$ is the Josephson constant and $R_K = h/e^2$ is the von Klitzing constant. For comparison purposes the 2006 and 2010 recommended values of h (open circles) are also shown. NML: National Measurement Institute, Australia; NPL: National Physical Laboratory, UK; PTB: Physikalisch-Technische Bundesanstalt, Germany; NIST: National Institute of Standards and Technology, USA; METAS: Federal Office of Metrology, Switzerland; IAC: International Avogadro Coordination (laboratories in various countries). Uncertainties are as published by groups and are intended to be one standard deviation estimates.

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as do some data compilations. The TGFC philosophy is highlighted in the proposed 2010 value and uncertainty of the Planck constant as shown in Fig. 1. The best value is mostly determined by two results that are discrepant by several standard uncertainties, the 2007 NIST watt balance result for the Planck constant, NIST-07 [25], and the 2011 International Avogadro Coordination project's determination of the Avogadro constant, IAC-11 [26]. However, the final 2010 CODATA uncertainty is not arbitrarily inflated to accommodate the discrepancy.

Second, unlike most key and inter-laboratory comparisons, where the same basic theories and experimental methods of physics are applied, an adjustment of the values of the fundamental constants relies on data from experiments utilizing widely differing underlying physical theories. For example, as shown in equations (1a), (1b), and (1c), various values of the fine-structure constant α are independently obtained through condensed matter physics and electrical metrology (1a), atomic physics and atom-recoil measurements (1b), and particle physics and quantum electrodynamics (QED) (1c):

$$R_K = \frac{h}{e^2} = \frac{\mu_0 c}{2\alpha} \tag{1a}$$

$$\frac{h}{m(X)} = \frac{\alpha^2 c}{2R_\infty} \frac{m_e}{m(X)} \tag{1b}$$

$$a_e = \sum_{n=1}^{\infty} C_e^{(2n)} \left(\frac{\alpha}{\pi}\right)^n + a_e(\text{had}) + a_e(\text{weak}) , \tag{1c}$$

where R_K is the von Klitzing constant, μ_0 is the magnetic constant (permeability of vacuum), α is the fine-structure constant, $m(X)$ is the mass of element X, R_∞ is the Rydberg constant, m_e is the electron mass, a_e is the electron magnetic moment anomaly, $C_e^{(2n)}$ are QED expansion coefficients, and a_e(had) and a_e(weak) are the hadronic and electroweak contributions

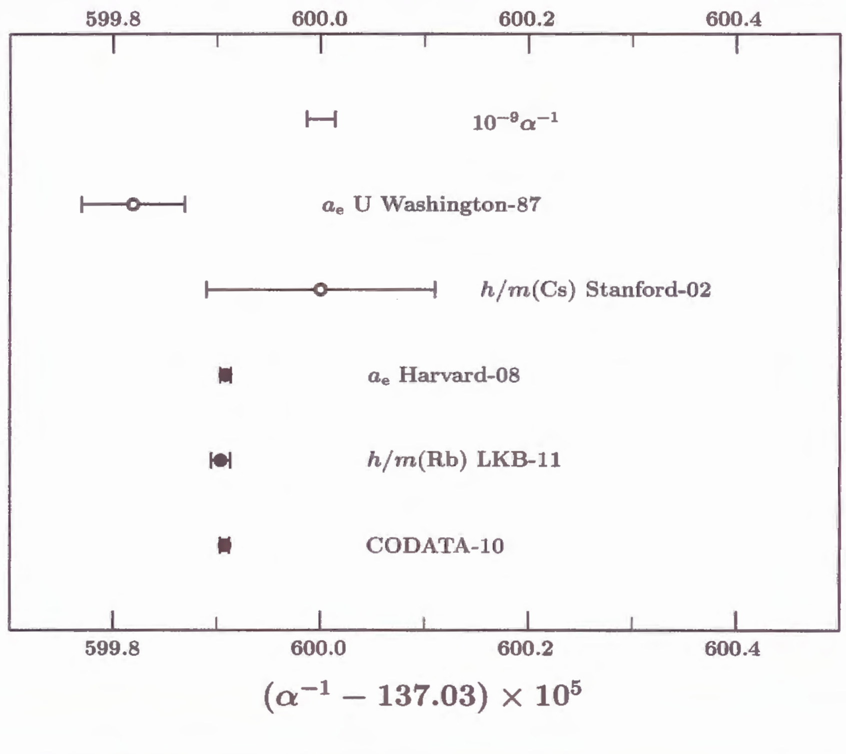

Figure 2. Input data related to the 2010 CODATA TGFC determination of the fine-structure constant. Data are from two electron magnetic moment anomaly measurements combined with QED theory, U Washington-87 and Harvard-08; and two atom-recoil experiments, Stanford-02 and LKB-11. However, the data in open circles did not meet the "self-sensitivity test" (see Section 3.2) and were not included in the final least-squares adjustment that determined the 2010 recommended values. For the same reason, data items NML-89, PTB-91, and METAS-11 in Fig. 1 were also omitted. U Washington: University of Washington, USA; Stanford: Stanford University, USA; Harvard: Harvard University, USA; LKB: Laboratoire Kastler-Brossel, France. Uncertainties are as published by groups and are intended to be one standard deviation estimates.

to a_e. Indeed, although the central role of the adjustment is to provide the best values of the fundamental constants (i.e., lowest uncertainties) to be used by researchers as they probe the laws of physics, an adjustment of this nature can also test the validity of the underlying physical theories themselves. However, unless otherwise indicated by the data, throughout an adjustment it is assumed the underlying physical theories are valid, such as special relativity, quantum mechanics, QED, the standard model of particle physics, including combined charge conjugation, parity inversion, time reversal (*CPT*) invariance, and the theory of the Josephson and quantum Hall effects.

Finally, also unlike most key and inter-laboratory comparisons, in some cases there is very limited redundancy so that one or two results dominate the final recommended value of a fundamental constant. Figure 2 shows the input data associated with experiments related to equations (1b) and (1c) in the determination of α for the 2010 adjustment, where the final value is dominated by the Harvard measurement of the electron magnetic moment anomaly [27] combined with QED theory [28]. This was also the case in the 2006 determination of the Boltzmann constant as shown in Fig. 3, where the final value was determined by the 1988 NIST acoustic gas thermometry (AGT) measurement, NIST-88 [29]. However in the intervening four years, there have been six new results that are highly consistent. The task group encourages researchers to continue their efforts relevant to the determination of the constants towards a data set as consistent as these and that will provide a firm basis for the values of h, e, k, and N_A chosen for the new SI.

3.1 Multivariate Least-Squares Analysis of the Data

The method presently used by the CODATA TGFC to evaluate relevant data is a multivariate least-squares analysis (LSA). The multivariate LSA

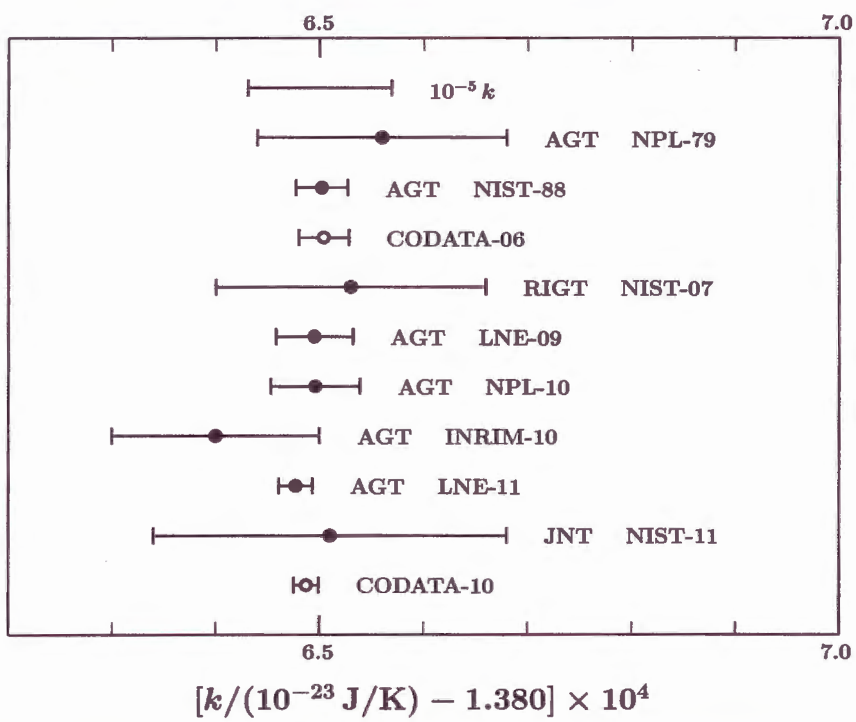

Figure 3. Input data related to the 2010 CODATA TGFC determination of the Boltzmann constant. Data are from six acoustic gas thermometry (AGT) experiments, NPL-79, NIST-88, LNE-09, NPL-10, INRIM-10, LNE-11; one refractive index gas thermometry (RIGT) experiment, NIST-07; and one Josephson noise thermometry (JNT) experiment, NIST-11. For comparison purposes the 2006 and 2010 recommended values of k (open circles) are also shown. The NIST-07 and NIST-11 data did not meet the "self-sensitivity test" (see Section 3.2) and were not included in the final least-squares adjustment that determined the 2010 recommended values. LNE: Laboratoire national de métrologie et d'essais, France; INRIM: Istituto Nazionale di Ricerca Metrologica, Italy. Uncertainties are as published by groups and are intended to be one standard deviation estimates.

is based on the fact that measured quantities, or input data, can be expressed as functions of fundamental constants. These expressions, or *observational equations*, are written in terms of a particular independent subset of the constants called *directly adjusted constants* (or for convenience simply *adjusted constants*). An example of observational equations, which are associated with the input data of Fig. 1, is:

$$K_{\mathrm{J}} = \left(\frac{8}{\mu_0 c}\right)\left[\frac{\alpha}{h}\right]^{1/2} \quad (2a)$$

$$K_{\mathrm{J}}^2 R_{\mathrm{K}} = \frac{4}{h} \quad (2b)$$

$$N_{\mathrm{A}} = \left(\frac{M_{\mathrm{u}}c}{2}\right)\frac{A_{\mathrm{r}}(\mathrm{e})\alpha^2}{R_\infty h}\,, \quad (2c)$$

where $K_{\mathrm{J}} = 2e/h$ is the Josephson constant, $M_{\mathrm{u}} = 0.001$ kg/mol exactly is the molar mass constant, and $A_{\mathrm{r}}(\mathrm{e})$ is the relative atomic mass of the electron. Observational equation (2a) has two input data for the measurement of K_{J}, one from a Hg electrometer, NML-89 [30], and another from a capacitor voltage balance, PTB-91 [31]; observational equation (2b) has five input data for the measurement of the product $K_{\mathrm{J}}^2 R_{\mathrm{K}}$ from five watt balances, NPL-90 [32], NIST-98 [33], NIST-07 [25], METAS-11 [34], and NPL-11 [35]; and observational equation (2c) has one input datum for the measurement of N_{A} from the International Avogadro Coordination project, IAC-11 [26]. There is no unique choice for the adjusted constants; however they must be chosen such that none can be expressed as a function of the others and the value of each is determined through some subset of the observational equations. The goal of the analysis is to find the values of the adjusted constants that predict values for the input data that best agree with the data themselves in the least-squares sense of a minimized variance. The remaining constants are then calculated from the adjusted constants. For example, of the four proposed constants to be defined as exact in the new SI, only h is an adjusted constant. The remaining three are calculated using the relations

$$e = \left(\frac{2\alpha h}{\mu_0 c}\right)^{1/2} \quad (3a)$$

$$k = \left(\frac{M_{\mathrm{u}}c}{2}\right) R \frac{A_{\mathrm{r}}(\mathrm{e})\alpha^2}{R_\infty h} \quad (3b)$$

$$N_{\mathrm{A}} = \left(\frac{M_{\mathrm{u}}c}{2}\right)\frac{A_{\mathrm{r}}(\mathrm{e})\alpha^2}{R_\infty h}\,, \quad (3c)$$

where R, the molar gas constant, is an adjusted constant, as are α, h, $A_{\mathrm{r}}(\mathrm{e})$, and R_∞. (Note that the quantities on the right-hand side of equations (3a), (3b), and (3c) are either adjusted constants or are exactly known.)

The least-squares method adopted follows that of Aitken [36] (see also Sheppard [37]) with the inverse variance weighting of each input datum and where correlations among input data are properly taken into account, as emphasized by Cohen [38]. Covariances are assigned to each pair of correlated input data based upon their uncertainty budgets. The CODATA 2010 set of recommended values is based on an final least-squares adjustment with $N = 163$ items of input data, $M = 86$ directly adjusted constants, and degrees of freedom $\nu = N - M = 77$. The statistic "chi-squared" for the adjustment is $\chi^2 = 59.1$ with probability $p(\chi^2|\nu) = 0.935$ and Birge ratio $R_{\mathrm{B}} = (\chi^2/\nu)^{1/2} = 0.876$.

3.2 The Determination of the Constants

The determination of the fundamental constants requires an iterative process and begins with a review of all available data for their mutual compatibility and their potential role in determining the recommended values of the constants, especially data that have become available since the last adjustment. The potential role of a particular datum is gauged by carrying out an initial multivariate LSA as described above using all available data to be considered. The consistency of the data is evaluated by directly comparing different measurements of the same quantity, and by directly comparing the values of a single fundamental constant inferred from measurements of different quantities as is shown in Figs. 1, 2, and 3. The statistic "chi-squared," χ^2, and the Birge ratio, R_{B}, are used to test the consistency of the data and the validity of inverse variance weighting. In general the normalized residuals of the analysis are used as a guide for relevant, but discrepant data, and expansion factors are applied to the weights of the discrepant data sub-sets such that the residuals of the analysis are at an acceptable level. With expansion factors applied, the multivariate LSA is performed again. The "self-sensitivity" coefficients of the data are then examined to determine if they have values greater than 0.01. Essentially, the uncertainty of an individual datum can be no more than about 10 times the uncertainty of the adjusted value of the input datum in order to be included in the final analysis. Figure 2 shows an example of input data that did not meet this criterion and were not included in the final adjustment (i.e., U Washington-87 and Stanford-02). A final multivariate LSA with the above evaluation criteria determines the directly adjusted constants and thus the recommended values and uncertainties of all of the fundamental constants.

4. New SI and the Future Role of the CODATA TGFC

When the available data are considered acceptable by the CIPM and CGPM for redefining the kilogram, ampere, kelvin, and mole in terms of exact values of h, e, k, and N_{A}, the CODATA TGFC is prepared to provide two special adjustments: one to determine the fixed values of h, e, k, and N_{A}; and a second to determine the remaining values and uncertainties of the other

Quantity	Symbol	Current SI u_r ($\times 10^{-9}$)	New SI u_r ($\times 10^{-9}$)
international prototype of the kilogram	$m(K)$	0	44
Planck constant	h	44	0
elementary charge	e	22	0
Boltzmann constant	k	910	0
Avogadro constant	N_A	44	0
molar gas constant	R	910	0
Faraday constant	F	22	0
Stefan-Boltzmann constant	σ	3600	0
electron mass	m_e	44	0.64
atomic mass constant	m_u	44	0.70
mass of ^{12}C	$m(^{12}C)$	44	0.70
molar mass of ^{12}C	$M(^{12}C)$	0	0.70
fine-structure constant	α	0.32	0.32
Josephson constant	K_J	22	0
von Klitzing constant	R_K	0.32	0
magnetic (permeability) constant	μ_0	0	0.32
electric (permittivity) constant	ε_0	0	0.32
vacuum impedance	Z_0	0	0.32
Planck charge	q_P	22	0.16
$E = mc^2$ energy equivalent	J↔kg	0	0
$E = hc/\lambda$ energy equivalent	J↔m^{-1}	44	0
$E = h\nu$ energy equivalent	J↔Hz	44	0
$E = kT$ energy equivalent	J↔K	910	0
1 J = 1 (C/e) eV energy equivalent	J↔eV	44	0

Table 1. Relative standard uncertainties, u_r, for a selection of fundamental constants and energy equivalents from the 2010 adjustment, in parts in 10^9. Note that u_r of $m(K)$ in the current SI is 0 only by definition. The new SI relative standard uncertainties assume fixed values of the Planck constant h, elementary charge e, Boltzmann constant k, and Avogadro constant N_A.

constants based upon the new definitions and available data. Table 1 shows the relative standard uncertainties, u_r, for a selection of fundamental constants and energy equivalents from the 2010 adjustment and the resulting u_r based on the new SI if the redefinition were to occur today. It is clear that all disciplines and research that rely on the values of the constants will be provided a better set of "tools" to continue expanding our understanding and knowledge of nature. After redefinition, the task group will continue the four year adjustment cycle to provide the user community with values of the constants having the smallest possible uncertainties consistent with the information available at the time.

5. References

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