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ON THE *CODATA* RECOMMENDED VALUES OF THE FUNDAMENTAL PHYSICAL CONSTANTS: V3.2(1998) & V4.0(2002)

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Abstract

Siver A.S., Ezhela V.V. On the CODATA Recommended Values of the Fundamental Physical Constants: V3.2(1998) & V4.0(2002): IHEP Preprint 2003–34. – Protvino, 2003. – p. 18, tables 12, refs.: 18.

With the help of special program package PAREVAL designed in *Mathematica* system we reproduce values of basic fundamental physical constants obtained by NIST and recommended by CODATA for international usage since 1998. In our adjustment we use the input data and methods published by NIST in 1998.

It is shown, that the detected earlier inaccuracy of published by NIST correlations (that made the NIST 1998&2002 results doubtful) are, most probably, due to inadmissible independent rounding.

The simple estimate of the critical numbers of decimal digits in the independently rounded correlation coefficients is obtained. Further independent rounding of "critically rounded" correlations can lead to the non positive semi definite correlation matrices and hence is inadmissable.

It is demonstrated by a few examples that the poor presentation of the correlated random quantities in the scientific literature is a common bad practice and is argued (once again) that the common standard for presentation numerical values of correlated quantities in publications and sites is urgently and badly needed.

Аннотация

Сивер А.С., Ежела В.В. О численных значениях фундаментальных физических постоянных, рекомендованных CODATA версий V3.2(1998) и V4.0(2002): Препринт ИФВЭ 2003–34. – Протвино, 2003. – 18 с., 12 табл., библиогр.: 18.

С помощью специального пакета программ PAREVAL, разработанного в системе *Mathematica*, воспроизведены значения базовых фундаментальных физических постоянных NIST, рекомендованных CODATA для международного использования с 1998 года. Показано, что обнаруженные ранее неточности значений коэффициентов корреляции погрешностей констант 1998 года обусловлены, скорее всего, их недопустимым независимым округлением. Коэффициенты корреляций погрешностей констант 2002 года также испорчены недопустимым округлением, и их нельзя использовать в высокоточных вычислениях.

Получена простая оценка критического числа десятичных знаков в значениях коэффициентов корреляции, дальнейшее независимое округление которых может приводить к потере положительной полуопределенности матрицы корреляций.

На нескольких примерах показано, что некорректное представление значений коррелированных случайных величин в публикациях — это распространенная вредная практика. Декларируется необходимость разработки и использования стандарта представления оценок коррелированных случайных величин в публикациях и на сайтах.

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1. Motivation

Fundamental physical constants (FPC) are the basic entities in pure and applied natural sciences and in technology. Thanks to efforts of many national metrology institutions, NIST[1] systematists, and international coordination by CODATA[2] we *seem* to have a more or less reliable procedures to monitor the development of the unified system of constants, their periodically adjusted numerical values, uncertainties, and correlations.

We use "*seem*" because in spite of many national and international documents on the rules and standards on the statistical and experimental data presentations in the official publications[3] there is a sharp contradiction between rules/standards and reality of scientific data exchanges in the past and modern scientific communication media.

An example of such contradictions is the lack of attention from producers (NIST) and overseers (CODATA) of the evaluated FPC data to the quality of the final data presentations in the official publications on the paper and even in electronic forms: data presented are incomplete and inaccurate as we will show further.

The other example of the mentioned contradiction is the ignorance of correlations in all respectable information resources: handbooks, textbooks, monographs, reviews, and scientific software packages that have reprinted samples of the recommended FPC-1998 (see, for example, [5] – [11]).

Since the release of FPC-1998 the scientific community obtained real access to the correlations of the FPC uncertainties and one can see that correlations between uncertainties of some universal constants are too "strong" to be ignored in high accuracy calculations. But unfortunately the correlation matrix presented on the NIST/CODATA site and reproduced partly in the publication [1] (see, Table XXV on the page 453) is non positive semi-definite in contradiction with definition of the correlation matrix. Looking at the NIST correlation coefficients one can see that they are rounded off too "tightly." Format of the numbers shows that they were rounded uniformly and independently (e.g. ignoring the crucial constraints that any covariance and correlation matrix must respect).

[1]National Institute of Standards and Technology (USA) [2].

[2]Committee on Data for Science and Technology [3].

[3]We failed, however, to find any official documents standardising the procedures of rounding average values, standard uncertainties, and their correlations of the **jointly measured or evaluated (adjusted)** quantities.

Table 1. Sample of a few NIST/CODATA:1998 recommended constants.

FPC name	Simbol [units]	Value (uncertainty)×scale	Correlations			
Elementary charge	e [C]	$1.602\,176\,462(63) \times 10^{-19}$	e	h	m_e	m_p
Planck constant	h [J s]	$6.626\,068\,76(52) \times 10^{-34}$	0.999			
Electron mass	m_e [kg]	$9.109\,381\,88(72) \times 10^{-31}$	0.990	0.996		
Proton mass	m_p [kg]	$1.672\,621\,58(13) \times 10^{-27}$	0.990	0.995	1.000	

From the textbooks on numerical calculations it is known that the rounding of the correlated values is subject of special treatment (see for example [12], page 499). The average values, standard uncertainties, and correlation coefficients could not be rounded off independently.

Independent rounding may lead to catastrophic changes in the connection of averages, standard uncertainties, and scatter ellipsoid: average values may get out of scatter ellipsoid, scatter ellipsoid may turn to hyperboloid after independent rounding off the correlation coefficients

With the lack of discussions of the rounding correlated quantities in the NIST/CODATA publications, we interpret this as the result of independent rounding that destroy catastrophically the system of adjusted values. An example of such catastrophe with FPC-1998 recommended for "public usage" is the negative variance for the Rydberg constant calculated from the equation $R_\infty = \alpha^2 m_e c/2h$ [13]. If this confusion did not caused by a misprint in sign of some correlation coefficient it is most probably the "inconsistency induced by rounding off" the adjusted FPC-1998.

If we are right in our account that corruption of the true data was due to independent rounding then we should clarify the influence of independent rounding of the average values and dispersions. To test this a reproduction of the whole adjustments procedure used by NIST experts is needed.

The main goal of this work is to reproduce the NIST results using their data and methods as they presented in their detailed publication [1] and on the NIST site and then to work out the proper way of correlated data presentation and exchange.

The other goal of our work is to draw attention (once again) of the physics community to the problem with standardization of the statistical (experimental) data presentation in the modern scientific communication media.

The rest of the paper is organized as follows. In the next section we present a few variants of our adjustment in comparison with corresponding NIST/CODATA results. The last section summarizes outputs from our exercises and our vision how to improve the situation.

2. On the NIST FPC Adjustments Technology

In our analyses we tried to be as close as possible to the NIST adjustments strategy. Fortunately more or less complete overview of the NIST:1998 adjustment procedure including detailed presentation of the experimental data, theoretical models and formulae, the FPC evaluation strategy description, and explanation of the specific aspects of the calculations were published in [1]. To test the **traceability** of the NIST results through their public information resources we have attempted to reproduce NIST FPC values on the basis of data, formulae and instructions from publication [1] and NIST site only.

Table 2. Basic adjusted constants.

	Symbol	FPC-1998 values V3.2	Connections
1	R_∞	10 973 731.568 549(83) m^{-1}	$R_\infty = \alpha^2 m_e c/2h$
2	$A_r(e)$	5.485 799 110(12) $\times 10^{-4}\,u$	
3	$A_r(p)$	1.007 276 466 88(13) u	
4	$A_r(n)$	1.008 664 915 78(55) u	
5	$A_r(d)$	2.013 553 212 71(35) u	
6	$A_r(h)$	3.014 932 234 69(86) u	
7	$A_r(\alpha)$	4.001 506 1747(10) u	
8	α	7.297 352 533(27) $\times 10^{-3}$	$\alpha = e^2/2\epsilon_0 hc$
9	μ_{e^-}/μ_p	−658.210 6875(66)	
10	μ_d/μ_e^-	−4.664 345 537(50) $\times 10^{-4}$	
11	μ_{e^-}/μ_p'	−658.227 5954(71)	
12	μ_h'/μ_p'	−0.761 786 1313(33)	
13	μ_n/μ_p'	−0.684 996 94(16)	
14	m_e/m_μ	4.836 332 10(15) $\times 10^{-3}$	
15	h	6.626 068 76(52) $\times 10^{-34}$ J s	
16	R	8.314 472(15) J $\mathrm{mol}^{-1}\,\mathrm{K}^{-1}$	
17	xu(Cu Kα_1)	1.002 077 03(28) $\times 10^{-13}$ m	λ(CuK$_{\alpha 1}$) = 1 573.400xu(Cu Kα_1)
18	xu(Mo Kα_1)	1.002 099 59(53) $\times 10^{-13}$ m	λ(MoK$_{\alpha 1}$) = 707.831xu(Mo Kα_1)
19	Å*	1.000 015 01(90) $\times 10^{-10}$ m	λ(WK$_{\alpha 1}$) = 0.2090100Å*
20	d_{220}(ILL)	not given	
21	d_{220}(N)	not given	
22	d_{220}(W17)	not given	
23	d_{220}(W04)	not given	
24	d_{220}(W4.2a)	not given	
25	d_{220}(MO*4)	not given	
26	d_{220}(SH1)	not given	
27	d_{220}	1.920 155 845(56) $\times 10^{-10}$ m	
28	R_p	0.907(32) $\times 10^{-15}$ m	From [1], page 440
29	R_d	2.153(14) $\times 10^{-15}$ m	From [1], page 440

There are 107 principal input data expressed as functions of 57 adjusted constants (variables) via the set of observational equations. These 57 variables are subdivided in two classes: constants (see **Table 2**) and corrections (see **Table 3**)

Numerical values in the Tables 2, 3 are presented in the standard concise form $X(Y) \times 10^Z$ u (where X — average value, Y — standard uncertainty of X referred to the last digits of the quoted value, u — unit) and are expressed in SI. The symbols of adjusted constants are as follows: R_∞ (Rydberg constant); α (fine structure constant); h (Plank constant); m_e/m_μ (electron-muon mass ratio); $A_r(X)$ (mass of the parcticle X in atomic units), where X denotes symbol of the particle, such as electron or alpha-particle; μ_X/μ_Y (X, Y magnetic moment ratio); R — molar gas constant; xu(X Kα_1) — x-ray unit of the X atom; d_{220}(X) — {220} lattice spacing of the different (X) silicon mono-crystal (d_{220}); R_p and R_d are the bound-state proton and deuteron rms charge radii.

Table 3. Basic adjusted corrections.

	NIST Symbol	NIST/CODATA:1998 Value	Comments
30	$\delta_H(1,0,1)$	not given	
31	$\delta_H(2,0,1)$	not given	
32	$\delta_H(3,0,1)$	not given	
33	$\delta_H(4,0,1)$	not given	
34	$\delta_H(6,0,1)$	not given	
35	$\delta_H(8,0,1)$	not given	
36	$\delta_H(2,1,1)$	not given	
37	$\delta_H(4,1,1)$	not given	
38	$\delta_H(2,1,3)$	not given	
39	$\delta_H(4,1,3)$	not given	
40	$\delta_H(8,2,3)$	not given	
41	$\delta_H(12,2,3)$	not given	
42	$\delta_H(4,2,5)$	not given	
43	$\delta_H(6,2,5)$	not given	
44	$\delta_H(8,2,5)$	not given	
45	$\delta_H(12,2,5)$	not given	
46	$\delta_D(1,0,1)$	not given	
47	$\delta_D(2,0,1)$	not given	
48	$\delta_D(4,0,1)$	not given	
49	$\delta_D(8,0,1)$	not given	
50	$\delta_D(8,2,3)$	not given	
51	$\delta_D(12,2,3)$	not given	
52	$\delta_D(4,2,5)$	not given	
53	$\delta_D(8,2,5)$	not given	
54	$\delta_D(12,2,5)$	not given	
55	δ_e	$0.1(1.1) \times 10^{-12}$	From [1], page 457
56	δ_{Mu}	not given	
57	δ_μ	$0.0(6.4) \times 10^{-10}$	From [1], page 457

There are also 28 adjusted variables (see Table 3) that are not fundamental at all, but were introduced in order to decrease the theoretical uncertainty of the several observational equations. They are: $\delta_{\mathrm{N}}(n, \mathrm{L}, 2 \cdot \mathrm{j})$ — additive correction to $n\mathrm{L_j}$ energy level of the hydrogen (N=H) and deuterium (N=D); δ_e, δ_μ — additive correction to electron and muon magnetic moment anomaly, δ_{Mu} — additive correction to hyperfine splitting of the muonium basic bound state.

Unfortunately the set of final values released so far by NIST/CODATA:1998 does not contain estimates for large part of the 57 adjusted variables (marked as "not given" in the Tables 2, 3 in cases when we failed to find corresponding output value on the site CODATA Fundamental Physical Constants. Version 3.2 Release date: 1 October 2003. [4]). Hence our comparison will be incomplete to this extent.

The other problem that makes the straightforward reproduction of the NIST estimates impossible is the corrupted presentation of the input correlation sub-matrix (see [1], page 434, Table XIV.A.2) of the data related to the Rydberg constant. It is non positive definite. We interpret this confusion as the result of unjustified independent rounding of correlation coefficients (motivated only to be convenient for publication on the paper). Fortunately the correlation sub-matrix for the other data presented in [1] (see page 436, Table XIV.B.2) is positive definite.

In spite of the incomplete presentation of the adjustment results and corrupted input correlation data we decided to clarify to what extent the ignorance of the input correlations in part or totally will modify the output constants, supposing that average values of the constants are correct as well as their standard uncertainties.

The strategy of comparisons is as follows. First of all we have convinced that the NIST method used to obtain values of adjustable variables is indeed the method to find stationary points of the "linearized" χ^2. If the input covariance matrix is positive definite then the obtained solution will be a minimum and adjustment will be stable if we turn lucky to get into vicinity of a global minimum. If the input covariance matrix is non positive definite then the task of finding stationary points could be solved for non-degenerate weight matrices but in this case the task has no connection with least squares method of constants estimation.

Nevertheless it is interesting to compare values of adjusted variables that can be obtained by NIST method in our PAREVAL package (from the NIST starting point in the adjusted variables space and with rounded by NIST input covariance matrix [1]) with true NIST/CODATA:1998 recommended values.

2.1. Calculations with input correlator published by NIST

Corresponding results are presented in **Table 4**, where in the fifth column the normalized difference of values of third X_3 and fourth X_4 columns is defined as follows

$$\Delta = \frac{X_3 - X_4}{\sqrt{\sigma^2(X_3) + \sigma^2(X_4)}}.$$

In our adjustment we use close to the NIST starting point (used for finding zero of the gradient of χ^2 in step-by-step method) in the adjusted variables space and "weights" were constructed from rounded by NIST input "correlation" matrix [1].

As it can be seen from the fifth column of the Table 4, the shifts in average values are in general well inside the ranges defined by the quadratically combined "uncertainties". In all tables, as a rule, we save in average values and corresponding uncertainties one more digit to show that some values are not reproduced exactly when rounding independently even if they are well inside the uncertainties ($|\Delta| < 0.1$).

Table 4. Comparison of the true NIST/CODATA:1998 recommended values (third column) with corresponding values (fourth column) that have been obtained at IHEP by the NIST method in our PAREVAL package.

	FPC Symbol	NIST:1998 Value NIST true correlator	IHEP:2003 Value NIST published correlator	Δ
1	R_∞	$1.097\,373\,156\,8549(83) \times 10^{7}$	$1.097\,373\,156\,854\,7(83) \times 10^{7}$	0.0153
2	$A_r(e)$	$5.485\,799\,110(12) \times 10^{-4}$	$5.485\,799\,1097(116) \times 10^{-4}$	0.0171
3	$A_r(p)$	$1.007\,276\,466\,88(13)$	$1.007\,276\,466\,883(132)$	−0.0153
4	$A_r(n)$	$1.008\,664\,915\,78(55)$	$1.008\,664\,915\,784(547)$	0.00501
5	$A_r(d)$	$2.013\,553\,212\,71(35)$	$2.013\,553\,212\,706(344)$	0.00833
6	$A_r(h)$	$3.014\,932\,234\,69(86)$	$3.014\,932\,234\,691(860)$	−0.001
7	$A_r(\alpha)$	$4.001\,506\,1747(10)$	$4.001\,506\,174\,69(100)$	0.00456
8	α	$7.297\,352\,533(27) \times 10^{-3}$	$7.297\,352\,5335(265) \times 10^{-3}$	−0.0132
9	μ_{e^-}/μ_p	$-6.582\,106\,875(66) \times 10^{2}$	$-6.582\,106\,8753(659) \times 10^{2}$	0.00375
10	μ_d/μ_e^-	$-4.664\,345\,537(50) \times 10^{-4}$	$-4.664\,345\,5371(500) \times 10^{-4}$	0.0009
11	μ_{e^-}/μ'_p	$-6.582\,275\,954(71) \times 10^{2}$	$-6.582\,275\,9549(717) \times 10^{2}$	0.00938
12	μ'_h/μ'_p	$-7.617\,861\,313(33) \times 10^{-1}$	$-7.617\,861\,3130(330) \times 10^{-1}$	6.64×10^{-9}
13	μ_n/μ'_p	$-6.849\,9694(16) \times 10^{-1}$	$-6.849\,969\,40(160) \times 10^{-1}$	6.16×10^{-12}
14	m_e/m_μ	$4.836\,332\,10(15) \times 10^{-3}$	$4.836\,332\,107(144) \times 10^{-3}$	−0.0360
15	h	$6.626\,068\,76(52) \times 10^{-34}$	$6.626\,068\,756(522) \times 10^{-34}$	0.00530
16	R	$8.314\,472(15)$	$8.314\,4724(147)$	−0.0214
17	xu(Cu Kα_1)	$1.002\,077\,03(28) \times 10^{-13}$	$1.002\,077\,021(287) \times 10^{-13}$	0.0212
18	xu(Mo Kα_1)	$1.002\,099\,59(53) \times 10^{-13}$	$1.002\,099\,593(516) \times 10^{-13}$	−0.00461
19	Å*	$1.000\,015\,01(90) \times 10^{-10}$	$1.000\,015\,010(901) \times 10^{-10}$	−0.000017
20	d_{220}(ILL)	not given	$1.920\,155\,8160(558) \times 10^{-10}$	— — —
21	d_{220}(N)	not given	$1.920\,155\,8191(508) \times 10^{-10}$	— — —
22	d_{220}(W17)	not given	$1.920\,155\,8411(484) \times 10^{-10}$	— — —
23	d_{220}(W04)	not given	$1.920\,155\,8103(520) \times 10^{-10}$	— — —
24	d_{220}(W4.2a)	not given	$1.920\,155\,7995(496) \times 10^{-10}$	— — —
25	d_{220}(MO*4)	not given	$1.920\,155\,6075(439) \times 10^{-10}$	— — —
26	d_{220}(SH1)	not given	$1.920\,155\,7624(463) \times 10^{-10}$	— — —
27	d_{220}	$1.920\,155\,845(56) \times 10^{-10}$	$1.920\,155\,8391(561) \times 10^{-10}$	0.0749
28	R_p	$0.907(32) \times 10^{-15}$	$0.9066(329) \times 10^{-16}$	— — —
29	R_d	$2.153(14) \times 10^{-15}$	$2.1528(137) \times 10^{-15}$	— — —
		$\chi^2/ndf = \mathbf{0.90}$ [1], page 446	$\chi^2/ndf = \mathbf{0.90}$	

As we have no NIST/CODATA:1998 final values of the adjusted corrections we compare our results with the input values which we use (follow NIST) as observational equation like $\delta = 0.0\ldots0(u(\delta))$ (see **Table 5**). We see that shifts in average values for all corrections are also well inside the intervals defined by the input estimates of theoretical systematic uncertainties.

Table 5. Comparison of the input NIST/CODATA:1998 va-lues (third column) with corresponding values (fourth column) that obtained at IHEP by the NIST method in our PAREVAL package.

	FPC Symbol	NIST:1998 input value	IHEP:2003 value NIST published correlator
30	$\delta_H(1,0,1)$	$0.0000(9.0000) \times 10^4$	$0.009(8.974) \times 10^4$
31	$\delta_H(2,0,1)$	$0.0000(1.1000) \times 10^4$	$0.007(1.097) \times 10^4$
32	$\delta_H(3,0,1)$	$0.000(3.300) \times 10^3$	$0.003(3.291) \times 10^3$
33	$\delta_H(4,0,1)$	$0.000(1.400) \times 10^3$	$0.009(1.396) \times 10^3$
34	$\delta_H(6,0,1)$	$0.00(4.20) \times 10^2$	$0.00(4.19) \times 10^2$
35	$\delta_H(8,0,1)$	$0.00(1.80) \times 10^2$	$0.00(1.79) \times 10^2$
36	$\delta_H(2,1,1)$	$0.000(1.100) \times 10^3$	$-0.04(1.09) \times 10^3$
37	$\delta_H(4,1,1)$	$0.00(1.40) \times 10^2$	$-0.05(1.39) \times 10^2$
38	$\delta_H(2,1,3)$	$0.000(1.100) \times 10^3$	$0.01(1.10) \times 10^3$
39	$\delta_H(4,1,3)$	$0.00(1.40) \times 10^2$	$0.02(1.39) \times 10^2$
40	$\delta_H(8,2,3)$	$0.0(1.7) \times 10^1$	$-0.00(1.70) \times 10^1$
41	$\delta_H(12,2,3)$	$0.0(5.0)$	$-0.007(5.000)$
42	$\delta_H(4,2,5)$	$0.00(1.40) \times 10^2$	$0.01(1.40) \times 10^2$
43	$\delta_H(6,2,5)$	$0.0(4.0) \times 10^1$	$0.03(4.00) \times 10^1$
44	$\delta_H(8,2,5)$	$0.0(1.7) \times 10^1$	$0.10(1.70) \times 10^1$
45	$\delta_H(12,2,5)$	$0.0(5.0)$	$0.04(5.00)$
46	$\delta_D(1,0,1)$	$0.0000(8.9000) \times 10^4$	$0.005(8.877) \times 10^4$
47	$\delta_D(2,0,1)$	$0.0000(1.1000) \times 10^4$	$0.001(1.097) \times 10^4$
48	$\delta_D(4,0,1)$	$0.000(1.400) \times 10^3$	$0.001(1.396) \times 10^3$
49	$\delta_D(8,0,1)$	$0.00(1.70) \times 10^2$	$0.00(1.70) \times 10^2$
50	$\delta_D(8,2,3)$	$0.0(1.1) \times 10^1$	$-0.00(1.10) \times 10^1$
51	$\delta_D(12,2,3)$	$0.0(3.4)$	$-0.00(3.40)$
52	$\delta_D(4,2,5)$	$0.0(9.2) \times 10^1$	$0.06(9.20) \times 10^1$
53	$\delta_D(8,2,5)$	$0.0(1.1) \times 10^1$	$0.008(1.100) \times 10^1$
54	$\delta_D(12,2,5)$	$0.0(3.4)$	$0.02(3.40)$
55	δ_e	$0.00(1.1) \times 10^{-12}$	$0.01(1.10) \times 10^{-12}$
56	δ_{Mu}	$0.00(1.20) \times 10^2$	$0.01(1.17) \times 10^2$
57	δ_μ	$0.0(6.4) \times 10^{-10}$	$0.00(6.40) \times 10^{-10}$
			$\boldsymbol{\chi^2/ndf = 0.90}$

2.2. Calculations with identity input correlation matrix

We learn from Tables 4 and 5 that rounded input correlation matrix leads to slightly shifted values of the basic constants and corrections that are well inside the uncertainties. To clarify the importance of correlations further and to test our package we produce adjustment ignoring input correlations.

Table 6. Comparison of the true NIST/CODATA:1998 recommended values (third column) with corresponding values (fourth column) that obtained at IHEP by the NIST method in our PAREVAL package. In this adjustment we use the same starting point as in previous run and weights were constructed completely ignoring input correlations. We see (from the fifth column) that shifts in average values are in general inside the quadratically combined "uncertainties".

	FPC Symbol	NIST:1998 Value NIST true correlator	IHEP:2003 Value Identity matrix correlator	Δ
1	R_∞	$1.097\,373\,156\,8549(83) \times 10^{7}$	$1.097\,373\,156\,8545(103) \times 10^{7}$	0.0314
2	$A_r(e)$	$5.485\,799\,110(12) \times 10^{-4}$	$5.485\,799\,1099(116) \times 10^{-4}$	0.00317
3	$A_r(p)$	1.007 276 466 88(13)	1.007 276 466 883(132)	−0.0138
4	$A_r(n)$	1.008 664 915 78(55)	1.008 664 915 774(556)	0.00731
5	$A_r(d)$	2.013 553 212 71(35)	2.013 553 212 688(360)	0.0439
6	$A_r(h)$	3.014 932 234 69(86)	3.014 932 234 690(860)	0.000402
7	$A_r(\alpha)$	4.001 506 1747(10)	4.001 506 17469(100)	0.00459
8	α	$7.297\,352\,533(27) \times 10^{-3}$	$7.297\,352\,5349(266) \times 10^{-3}$	−0.0500
9	μ_{e^-}/μ_p	$-6.582\,106\,875(66) \times 10^{2}$	$-6.582\,106\,8754(659) \times 10^{2}$	0.00432
10	μ_d/μ_{e^-}	$-4.664\,345\,537(50) \times 10^{-4}$	$-4.664\,345\,5371(500) \times 10^{-4}$	0.000901
11	μ_{e^-}/μ'_p	$-6.582\,275\,954(71) \times 10^{2}$	$-6.582\,275\,9550(717) \times 10^{2}$	0.00973
12	μ'_h/μ'_p	$-7.617\,861\,313(33) \times 10^{-1}$	$-7.617\,861\,3130(330) \times 10^{-1}$	6.64×10^{-9}
13	μ_n/μ'_p	$-6.849\,9694(16) \times 10^{-1}$	$-6.849\,96940(160) \times 10^{-1}$	6.16×10^{-12}
14	m_e/m_μ	$4.836\,332\,10(15) \times 10^{-3}$	$4.836\,332\,103(142) \times 10^{-3}$	−0.0124
15	h	$6.626\,068\,76(52) \times 10^{-34}$	$6.626\,068\,756(522) \times 10^{-34}$	0.00523
16	R	8.314 472(15)	8.314 4724(147)	−0.0214
17	xu(Cu Kα_1)	$1.002\,077\,03(28) \times 10^{-13}$	$1.002\,077\,018(288) \times 10^{-13}$	0.0306
18	xu(Mo Kα_1)	$1.002\,099\,59(53) \times 10^{-13}$	$1.002\,099\,596(516) \times 10^{-13}$	−0.00803
19	Å*	$1.000\,015\,01(90) \times 10^{-10}$	$1.000\,015\,013(901) \times 10^{-10}$	−0.00200
20	d_{220}(ILL)	not given	$1.920\,155\,8093(517) \times 10^{-10}$	— — —
21	d_{220}(N)	not given	$1.920\,155\,8239(635) \times 10^{-10}$	— — —
22	d_{220}(W17)	not given	$1.920\,155\,8380(545) \times 10^{-10}$	— — —
23	d_{220}(W04)	not given	$1.920\,155\,8102(460) \times 10^{-10}$	— — —
24	d_{220}(W4.2a)	not given	$1.920\,155\,7910(563) \times 10^{-10}$	— — —
25	d_{220}(MO*4)	not given	$1.920\,155\,5957(457) \times 10^{-10}$	— — —
26	d_{220}(SH1)	not given	$1.920\,155\,7631(509) \times 10^{-10}$	— — —
27	d_{220}	$1.920\,155\,845(56) \times 10^{-10}$	$1.920\,155\,8390(506) \times 10^{-10}$	0.0800
28	R_p	$0.907(32) \times 10^{-15}$	$0.9087(261) \times 10^{-15}$	— — —
29	R_d	$2.153(14) \times 10^{-15}$	$2.1519(115) \times 10^{-15}$	— — —
		$\chi^2/ndf = 0.90$ [1], page 446	$\chi^2/ndf = 0.84$	

Table 7. Comparison of the obtained values of additive corrections with input estimates of the theoretical systematic uncertainties.

	FPC Symbol	NIST:1998 input value	IHEP:2003 value Identity matrix correlator
30	$\delta_H(1,0,1)$	$0.0000(9.0000) \times 10^4$	$-0.06(6.40) \times 10^4$
31	$\delta_H(2,0,1)$	$0.0000(1.1000) \times 10^4$	$-0.07(7.96) \times 10^3$
32	$\delta_H(3,0,1)$	$0.000(3.300) \times 10^3$	$0.01(3.29) \times 10^3$
33	$\delta_H(4,0,1)$	$0.000(1.400) \times 10^3$	$0.01(1.39) \times 10^3$
34	$\delta_H(6,0,1)$	$0.00(4.20) \times 10^2$	$0.02(4.20) \times 10^2$
35	$\delta_H(8,0,1)$	$0.00(1.80) \times 10^2$	$-0.01(1.80) \times 10^2$
36	$\delta_H(2,1,1)$	$0.000(1.100) \times 10^3$	$-0.05(1.10) \times 10^3$
37	$\delta_H(4,1,1)$	$0.00(1.40) \times 10^2$	$0.01(1.40) \times 10^2$
38	$\delta_H(2,1,3)$	$0.000(1.100) \times 10^3$	$0.03(1.10) \times 10^3$
39	$\delta_H(4,1,3)$	$0.00(1.40) \times 10^2$	$-0.02(1.40) \times 10^2$
40	$\delta_H(8,2,3)$	$0.0(1.7) \times 10^1$	$0.00(1.70) \times 10^1$
41	$\delta_H(12,2,3)$	$0.0(5.0)$	$-0.00(5.00)$
42	$\delta_H(4,2,5)$	$0.00(1.40) \times 10^2$	$0.005(1.400) \times 10^2$
43	$\delta_H(6,2,5)$	$0.0(4.0) \times 10^1$	$-0.009(4.000) \times 10^1$
44	$\delta_H(8,2,5)$	$0.0(1.7) \times 10^1$	$0.000(1.700) \times 10^1$
45	$\delta_H(12,2,5)$	$0.0(5.0)$	$-0.00(5.00)$
46	$\delta_D(1,0,1)$	$0.0000(8.9000) \times 10^4$	$0.05(6.50) \times 10^4$
47	$\delta_D(2,0,1)$	$0.0000(1.1000) \times 10^4$	$-0.04(8.07) \times 10^3$
48	$\delta_D(4,0,1)$	$0.000(1.400) \times 10^3$	$-0.08(1.40) \times 10^3$
49	$\delta_D(8,0,1)$	$0.00(1.70) \times 10^2$	$0.02(1.70) \times 10^2$
50	$\delta_D(8,2,3)$	$0.0(1.1) \times 10^1$	$-0.00(1.10) \times 10^1$
51	$\delta_D(12,2,3)$	$0.0(3.4)$	$-0.00(3.40)$
52	$\delta_D(4,2,5)$	$0.0(9.2) \times 10^1$	$0.00(9.20) \times 10^1$
53	$\delta_D(8,2,5)$	$0.0(1.1) \times 10^1$	$0.00(1.10) \times 10^1$
54	$\delta_D(12,2,5)$	$0.0(3.4)$	$-0.00(3.40)$
55	δ_e	$0.0(1.1) \times 10^{-12}$	$0.08(1.10) \times 10^{-12}$
56	δ_{Mu}	$0.00(1.20) \times 10^2$	$0.01(1.17) \times 10^2$
57	δ_μ	$0.0(6.4) \times 10^{-10}$	$0.00(6.40) \times 10^{-10}$
			$\boldsymbol{\chi^2/ndf = 0.84}$

Now we can compare values of constants and corrections obtained with rounded correlator and without correlations (see **Tables 8, 9**).

Table 8. Comparison of constant estimates obtained with NIST published input correlations and with identity matrix as input correlation matrix.

	FPC Symbol	IHEP:2003 value NIST published correlator	IHEP:2003 Value Identity matrix correlator	Δ
1	R_∞	$1.097\,373\,156\,855(8) \times 10^{7}$	$1.097\,373\,156\,854(10) \times 10^{7}$	0.018
2	R_p	$9.066(329) \times 10^{-16}$	$9.087(261) \times 10^{-16}$	−0.048
3	R_d	$2.1528(137) \times 10^{-15}$	$2.1519(115) \times 10^{-15}$	0.048
4	$A_r(e)$	$5.485\,799\,1097(116) \times 10^{-4}$	$5.485\,799\,1099(116) \times 10^{-4}$	−0.014
5	$A_r(p)$	$1.007\,276\,466\,883(132)$	$1.007\,276\,466\,883(132)$	0.0015
6	$A_r(n)$	$1.008\,664\,915\,784(547)$	$1.008\,664\,915\,774(566)$	0.012
7	$A_r(d)$	$2.013\,553\,212\,706(344)$	$2.013\,553\,212\,688(360)$	0.036
8	$A_r(h)$	$3.014\,932\,234\,691(860)$	$3.014\,932\,234\,690(860)$	0.0014
9	$A_r(\alpha)$	$4.001\,506\,174\,69(100)$	$4.001\,506\,174\,69(100)$	0.000 33
10	α	$7.297\,352\,5335(265) \times 10^{-3}$	$7.297\,352\,5349(266) \times 10^{-3}$	−0.037
11	μ_{e^-}/μ_p	$-6.582\,106\,8753(659) \times 10^{2}$	$-6.582\,106\,8754(659) \times 10^{2}$	0.0058
12	μ_d/μ_e^-	$-4.664\,345\,5371(500) \times 10^{-4}$	$-4.664\,345\,5371(500) \times 10^{-4}$	0
13	μ_{e^-}/μ'_p	$-6.582\,275\,9549(717) \times 10^{2}$	$-6.582\,275\,9550(717) \times 10^{2}$	0.0035
14	μ'_h/μ'_p	$-7.617\,861\,3130(330) \times 10^{-1}$	$-7.617\,861\,3130(330) \times 10^{-1}$	0
15	μ_n/μ'_p	$-6.849\,969\,40(160) \times 10^{-1}$	$-6.849\,969\,40(160) \times 10^{-1}$	0
16	m_e/m_μ	$4.836\,332\,107(144) \times 10^{-3}$	$4.836\,332\,103(142) \times 10^{-3}$	0.024
17	h	$6.626\,068\,756(522) \times 10^{-34}$	$6.626\,068\,756(522) \times 10^{-34}$	−0.000 64
18	R	$8.314\,4724(147)$	$8.314\,4724(147)$	0
19	xu(Cu Kα_1)	$1.002\,077\,021(287) \times 10^{-13}$	$1.002\,077\,018(288) \times 10^{-13}$	0.0093
20	xu(Mo Kα_1)	$1.002\,099\,593(516) \times 10^{-13}$	$1.002\,099\,596(516) \times 10^{-13}$	−0.0035
21	Å*	$1.000\,015\,010(901) \times 10^{-10}$	$1.000\,015\,013(901) \times 10^{-10}$	−0.0020
22	d_{220}(ILL)	$1.920\,155\,8160(558) \times 10^{-10}$	$1.920\,155\,8093(517) \times 10^{-10}$	0.087
23	d_{220}(N)	$1.920\,155\,8191(508) \times 10^{-10}$	$1.920\,155\,8239(635) \times 10^{-10}$	−0.060
24	d_{220}(W17)	$1.920\,155\,8411(484) \times 10^{-10}$	$1.920\,155\,8380(545) \times 10^{-10}$	0.043
25	d_{220}(W04)	$1.920\,155\,8103(520) \times 10^{-10}$	$1.920\,155\,8102(460) \times 10^{-10}$	0.0015
26	d_{220}(W4.2a)	$1.920\,155\,7995(496) \times 10^{-10}$	$1.920\,155\,7910(563) \times 10^{-10}$	0.011
27	d_{220}(MO*4)	$1.920\,155\,6075(439) \times 10^{-10}$	$1.920\,155\,5957(457) \times 10^{-10}$	0.019
28	d_{220}(SH1)	$1.920\,155\,7624(463) \times 10^{-10}$	$1.920\,155\,7631(509) \times 10^{-10}$	−0.0096
29	d_{220}	$1.920\,155\,8391(561) \times 10^{-10}$	$1.920\,155\,8390(506) \times 10^{-10}$	0.0013
		$\chi^2/ndf = 0.90$	$\chi^2/ndf = 0.84$	

Table 9. Comparison of correction estimates obtained with NIST published input correlations and with identity matrix as input correlation matrix.

	FPC Symbol	IHEP:2003 value NIST published correlator	IHEP:2003 Value Identity matrix correlator	Δ
30	$\delta_H(1,0,1)$	$0.009(8.974) \times 10^4$	$-0.062(6.40) \times 10^4$	0.057
31	$\delta_H(2,0,1)$	$0.007(1.0974) \times 10^4$	$-0.067(7.96) \times 10^3$	0.050
32	$\delta_H(3,0,1)$	$0.003(3.291) \times 10^3$	$0.012(3.29) \times 10^3$	-0.024
33	$\delta_H(4,0,1)$	$0.009(1.3963) \times 10^3$	$0.014(1.39) \times 10^3$	-0.069
34	$\delta_H(6,0,1)$	$0(4.19) \times 10^2$	$0.02(4.20) \times 10^2$	-0.0027
35	$\delta_H(8,0,1)$	$0(1.79) \times 10^2$	$-0.01(1.80) \times 10^2$	0.0056
36	$\delta_H(2,1,1)$	$-0.04(1.09) \times 10^3$	$-0.05(1.10) \times 10^3$	0.0069
37	$\delta_H(4,1,1)$	$-0.05(1.39) \times 10^2$	$0.01(1.40) \times 10^2$	-0.032
38	$\delta_H(2,1,3)$	$0.01(1.10) \times 10^3$	$0.03(1.10) \times 10^3$	-0.011
39	$\delta_H(4,1,3)$	$0.02(1.39) \times 10^2$	$-0.02(1.40) \times 10^2$	0.019
40	$\delta_H(8,2,3)$	$-0(1.70) \times 10^1$	$0(1.70) \times 10^1$	-0.0013
41	$\delta_H(12,2,3)$	$-0.007(5.000)$	$-0(5.00)$	-0.0060
42	$\delta_H(4,2,5)$	$0.01(1.400) \times 10^2$	$0.005(1.400) \times 10^2$	0.0024
43	$\delta_H(6,2,5)$	$0.03(4.00) \times 10^1$	$-0.009(4.000) \times 10^1$	0.0065
44	$\delta_H(8,2,5)$	$0.01(1.70) \times 10^1$	$0(1.70) \times 10^1$	0.0030
45	$\delta_H(12,2,5)$	$0.04(5.00)$	$-0(5.00)$	0.0053
46	$\delta_D(1,0,1)$	$0.0049(8.8767) \times 10^4$	$0.046(6.50) \times 10^4$	-0.041
47	$\delta_D(2,0,1)$	$0.0011(1.0970) \times 10^4$	$-0.04(8.07) \times 10^3$	0.0034
48	$\delta_D(4,0,1)$	$0.001(1.396) \times 10^3$	$-0.08(1.40) \times 10^3$	0.043
49	$\delta_D(8,0,1)$	$0(1.70) \times 10^2$	$0.02(1.70) \times 10^2$	-0.0076
50	$\delta_D(8,2,3)$	$-0(1.10) \times 10^1$	$0(1.10) \times 10^1$	-0.0012
51	$\delta_D(12,2,3)$	$-0(3.40)$	$-0(3.40)$	-0.0080
52	$\delta_D(4,2,5)$	$0.06(9.20) \times 10^1$	$0(9.20) \times 10^1$	0.0045
53	$\delta_D(8,2,5)$	$0.008(1.100) \times 10^1$	$0(1.10) \times 10^1$	0.0039
54	$\delta_D(12,2,5)$	$0.02(3.40)$	$-0(3.40)$	0.0052
55	δ_e	$0.010(1.10) \times 10^{-12}$	$0.08(1.10) \times 10^{-12}$	0.0091
56	δ_{Mu}	$0.013(1.17) \times 10^2$	$0.012(1.17) \times 10^2$	0.0058
57	δ_μ	$0(6.40) \times 10^{-10}$	$0(6.40) \times 10^{-10}$	0.000 20
		$\boldsymbol{\chi^2/ndf = 0.90}$	$\boldsymbol{\chi^2/ndf = 0.84}$	

Finally we have checked if the procedure to find minimum of the corresponding χ^2 without linearization of the observational equations used gives the same result. We have used the built-in *Mathematica* module to find minimum starting from the point in the adjusted variables space where the values of all 29 constants were taken as recommended by NIST/CODATA:1998 and the values of the rest 28 δ-corrections were taken as $0.001 \times u(\delta_{theor})$.

Corresponding value of $\chi^2/ndf = 0.84$, i.e. the same as obtained by using NIST procedure with linearization. Average values of the constants and corrections obtained by two different methods and different programs are practically the same (the maximal normalized difference is $|\Delta|_{max} \sim 10^{-21}$).

Our results lead us to the conclusion that NIST experts have used input correlation matrix close to that of presented in their published report. The fact that output correlation matrix is also non positive semi-definite does not allow one to exclude possibility that this non positive semi-definiteness could be induced by the non positive definiteness of the input matrix. This point remains to be clarified.

Let us compare a sample of our output correlation coefficients with corresponding NIST values.

Table 10. The values in bold are extracted from the NIST site whereas the values placed under main diagonal are our values obtained with no input correlations.

	R_∞	α	m_e/m_μ	h
R_∞	1.00	**−0.020**	**0.004**	**−0.000**
α	−0.0112	1.00	**−0.233**	**0.002**
m_e/m_μ	0.00235	−0.236	1.00	**−0.000**
h	−0.0000195	0.00174	−0.000410	1.00

As shown in the **Table 10** some of our correlation coefficients differ significantly from those of published by NIST.

Now we proceed to the general comments on the practice in the scientific literature and on the sites, where the correlated estimates of the random quantities jointly measured or evaluated are presented.

Often authors of the original papers appear to ignore correlations at all or to present them in an incomplete manner. So, it is hard to understand what type of uncertainties the quoted correlation matrix is referred to: statistical, systematic or total. It is dangerous (or even inadmissable) to use such incomplete data in further analyses and especially in the theory tests. Sometimes this incompleteness is caused by the too firm editors and publishers requirements. On the other hand there are also experimental mistakes (see examples of such situation in nuclear physics and technology [17]).

2.3. On the rounding off the correlated estimates

As it is well known the covariance matrix for the jointly estimated statistical quantities is by definition a positive semi-definite Hermitian matrix. It has real and nonnegative eigenvalues. The non degenerate correlation matrix is positive definite by definition.

Unfortunately some authors publish the "correlation matrix" with no final check up this crucial property of the correlation matrix. In majority cases it happens under the pressure of the limited publication space. So, authors are forced to present rounded correlation coefficients making this in an inadmissable manner. The rounding correlation coefficients off produced independently, saving symmetry of the matrix but ignoring such crucial properties as positive definiteness and positive semi-definiteness.

To be specific we quote a few examples from different subject fields. The first most striking example is yet discussed concerning the NIST publications on the adjusted fundamental constants, including the NIST site. The published version of the input correlation sub-matrix used to construct the weight matrix in their version of least squares method (LSM) is non positive definite, (see [1], page 434, Table XIV.A.2), it has two negative eigenvalues. Also the published version of the correlation sub-matrix between uncertainties in the recommended values of a sample of fundamental constants (see [1], page 453, Table XXV) is non positive semi-definite. We have convinced that it is because of poor accuracy of the presentation caused by unjustified uniform independent rounding of the correlation coefficients. Unfortunately the same way of presentation is used by NIST and approved by CODATA on their sites.

The other example is the publication of the CLEO collaboration on the high precision measurements of the τ-lepton decay branching ratios [14]. The final version of the correlation matrix presented in the Erratum is as follows:

Table 11. Correlation coefficients between branching fraction measurements of some τ-lepton decays from [14] .

τ	B_e	B_μ	B_h	B_μ/B_e	B_h/B_e
B_e	1.00	0.50	0.48	−0.42	−0.39
B_μ		1.00	0.50	0.58	0.08
B_h			1.00	0.07	0.63
B_μ/B_e				1.00	0.45
B_h/B_e					1.00

The corresponding eigenvalues are as follows:

$$2.173\,46, \quad 1.781\,87, \quad 1.054\,97, \quad -0.007\,491\,53, \quad -0.002\,803\,4$$

This confusion could be due to improper rounding, but we failed to show this by playing with numbers (de-rounding). The problem seems to be deeper and hence the CLEO data are questionable. These should be used with great caution in theory tests and in derivations of "world averaged" τ-lepton branching ratios.

As we already mentioned, the proper rounding procedure for the jointly measured or estimated quantities (average vector components, corresponding vector of their standard uncertainties, and correlation matrix) is the subject of special treatment. So it will be presented elsewhere if we will not found relevant papers published.

In the next section we construct a simple but important estimate of the threshold accuracy of the correlation coefficients that should not be violated while uniform independent rounding of correlation matrix elements.

3. On the numerical presentations of correlated quantities in computer readable files and in publications

Here we derive a simple sufficient estimate on the accuracy of a safely independent and uniform rounding the correlation matrix elements off.

Let A_{ij} be the $n \times n$ correlation matrix. It is real, symmetric, positive definite, and has matrix elements bounded as follows

$$A_{ii} = 1 \quad \text{for all} \quad i = 1, \ldots, n \quad \text{and} \quad |A_{i \neq j}| < 1.0.$$

Let B_{ij} be the "rounder" matrix, such that if it is added to the matrix A_{ij} the obtained matrix $G_{ij} = A_{ij} + B_{ij}$ will be real, symmetric, positive definite and all $|G_{i \neq j}| < 1$ are decimal numbers with k digits after the decimal point.

It is easy to see that matrix B_{ij} should have the following properties:

$$B_{ii} = 0 \quad \text{for all} \quad i = 1, \ldots, n \quad \text{and} \quad |B_{i \neq j}| \leq 5.0 \times 10^{-k-1}.$$

Let further $\alpha_1 \leq \cdots \leq \alpha_n$, $\beta_1 \leq \cdots \leq \beta_n$, and $\gamma_1 \leq \cdots \leq \gamma_n$ be the ordered sets of eigenvalues of the matrices A_{ij}, B_{ij}, and G_{ij} correspondingly. Then from the Weil's theorem for any $l = 1, \ldots, n$ we have the following inequalities [15],[16]:

$$\alpha_l + \beta_1 \leq \gamma_l \leq \alpha_l + \beta_n.$$

From the Gershgorin's theorem on the distributions of the eigenvalues of the Hermitian matrices [15] it follows that

$$\beta_1 \geq -(n-1) \cdot 5 \cdot 10^{-(k+1)} = -\frac{(n-1)}{2} \cdot 10^{-k}$$

and hence to have the matrix G_{ij} as positive semi definite matrix it is sufficient to demand

$$0 \leq \alpha_1 - \frac{(n-1)}{2} \cdot 10^{-k} \leq \gamma_1.$$

From the left inequality we have the final estimate for the threshold accuracy index for safely uniform independent rounding (SUIR) of the positive definite correlation matrix A_{ij} with minimal eigenvalue α_{min}

$$\boldsymbol{k \geq K^{th}_{\mathrm{SUIR}} = \left\lceil \log_{10} \left(\frac{n-1}{2 \cdot \alpha_{min}} \right) \right\rceil.} \tag{1}$$

NOTE. According to the Weil's theorem any uniform rounding the off-diagonal matrix elements of the positive semi-definite covariance matrix is forbidden.

Indeed, as rounder matrix is traceless Hermitian matrix, it obliged to have the negative minimal eigenvalue. Furthermore from the left inequality of the Weil's theorem statement it follows that any rounding could lead to the matrix with negative minimal eigenvalue.

This note shows that the special rounding strategy should be developed[4] for such covariance matrices as well as for the badly conditioned covariance matrices.

[4]We realise that, most probably, such a strategy was developed already somewhere, but unfortunately is deeply hidden in the national and international metrology instructions. Some relevant information see, for example, in the review [17], where the analogous concerns are expressed.

Now we can make a further comments on the values of the FPC correlation coefficients. In the Table 10, to simplify comparison with NIST data, our output correlation coefficients for basic FPC are presented with independent rounding to three significant digits. In fact we have minimal eigenvalue for our output 57×57 correlation matrix

$$\alpha_{min} = 1.290\,020\,861\,518\,11 \times 10^{-6}$$

and from the expression (1) for the critical accuracy it follows that *at least 8 digits after decimal point should be saved, when rounding uniformly and independently, to preserve positive definiteness of the output correlation matrix for basic sample of FPC.*

Table 12. Comparison of a few CODATA:1998 and CODATA:2002 recommended constants.

CODATA:1998	Simbol [units]		Value (uncertainty)×scale	Correlations			
Elementary charge	e	[C]	$1.602\,176\,462(63) \times 10^{-19}$	e	h	m_e	m_p
Planck constant	h	[J s]	$6.626\,068\,76(52) \times 10^{-34}$	0.999			
Electron mass	m_e	[kg]	$9.109\,381\,88(72) \times 10^{-31}$	0.990	0.996		
Proton mass	m_p	[kg]	$1.672\,621\,58(13) \times 10^{-27}$	0.990	0.995	1.000	
CODATA:2002	**Simbol [units]**		**Value (uncertainty)×scale**	**Correlations**			
Elementary charge	e	[C]	$1.602\,176\,53(14) \times 10^{-19}$	e	h	m_e	m_p
Planck constant	h	[J s]	$6.626\,0693(11) \times 10^{-34}$	1.000			
Electron mass	m_e	[kg]	$9.109\,3826(16) \times 10^{-31}$	0.998	0.999		
Proton mass	m_p	[kg]	$1.672\,621\,71(29) \times 10^{-27}$	0.998	0.999	1.000	

Eigenvalues of these correlation sub-matrices are as follows:

$$CODATA: 1998 \quad \{3.985, 0.0150769, 0.00536526, -0.000617335\};$$

$$CODATA: 2002 \quad \{3.997, 0.00315831, -0.000158432, -2.83681 \times 10^{-16}\}.$$

Both matrix are non positive semi-definite, the 2002 sub-matrix is degenerate as it is seen from the table above.

Another concern is the accuracy of data presentation on average values and standard uncertainties. As a rule 2002–uncertainties are more than two times larger than corresponding 1998-numbers (see the table above).

It is to some extent unexpected as the NIST bibliography database on FPC contains 528 additional to 1998 database entries classified as "experimental" and "original research" dated between 1999 and 2002 inclusively. Unfortunately the reasons of these enlargements of the standard uncertainties compared to the V3.2(1998)–release did not commented in the V4.0(2002)–release notification.

4. Conclusions

In this section we summarize the main results obtained and the discussions presented above.

- The *Mathematica* package PAREVAL was created and applied for adjustments of FPC. It reproduces the NIST/CODATA adjustment technology from their data and methods (as of 1998). It is composed of a few modules to maintain: the library of theoretical models, the experimental data compilation; to perform FPC evaluations, and for results presentation. The detailed package description as well as the address for access will be presented elsewhere [18].
- With the help of PAREVAL it is shown, that the "CODATA recommended values of the fundamental physical constants: 1998" V3.2 and "CODATA recommended values of the fundamental physical constants: 2002" V4.0 are questionable in, at least, the values of published correlation coefficients released in the NIST/CODATA sites. Most probably data were corrupted by unjustified rounding up the output values.

  It is argued that the released so far correlation coefficients are useful only to show the sizes of correlations but should not be used in the real calculations of high precision observables. It will be extremely useful if the released for the first time ASCII file be accompanied with easy computer readable files with the compact standardized names, units, average values, standard uncertainties and correlations presented as accurate as possible, without unjustified rounding up.
- The simple estimate for the threshold accuracy sufficient for safely uniform independent rounding of the positive definite correlation matrix is constructed. This estimate can be used to trigger the data corrupted by unjustified rounding.
- It is argued that it is an urgent need to create a common standard strategy of rounding interrelated quantities and common standard data structures to store and exchange the correlated data in the computation media. These standards should be freely available for science, education and technology practitioners.
  It seems that it is a real challenge to IT professionals to construct a flexible and tractable technology to handle large samples of correlated data which will preserve all global properties and interconnections of the principal components of the stricture in all data transformations and exchanges.

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The warning in the preface or in the caption of the FPC table noting that the uncertainties of some fundamental constants are highly correlated would be very useful.

[6] K. Hagiwara *et al.* [Particle Data Group Collaboration], "Review of Particle Physics", Phys. Rev. D **66** (2002) 010001.

The warning in the preface or in the caption of the FPC table noting that the uncertainties of some fundamental constants are highly correlated would be very useful.

[7] [Editors], "Fundamental physical constants (1998)" (in Russian).
Uspekhi Fizicheskikh Nauk **173** (2003) 339.

The warning in the preface or in the caption of the FPC table noting that the uncertainties of some fundamental constants are highly correlated would be very useful.

[8] http://library.wolfram.com/howtos/constants/.

It was a surprise to learn that system operates only with central values of FPC ignoring uncertainties and correlations.

[9] http://www.mapleapps.com/categories/maple8/html/scientificconstants.html.

Unfortunately there are no references to the sources of the FPC data on these pages.

[10] V. McLine (editor), BNL-NCS-44945-01/04-Rev. Informal Report ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6 (see: APPENDIX H. Recommended values of Physical Constants to be used in ENDF).

It was a surprise to learn that in the recommendations in the tables quoting some FPC values from CODATA the corresponding uncertainties and correlations are absent. Also it seems that in the high precision sector of nuclear physics, physicists should not ignore correlations of used FPC. So, the warning noting that the uncertainties of some fundamental constants are highly correlated would be very useful in the APPENDIX H.

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