WGFS 2021 adjustment of standard frequencies: Accounting for correlations due to the access to the SI second

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The WGFS subgroup worked over 2020-2021 to carry out the computation of the 2021 list of recommended frequencies (see https://www.bipm.org/en/publications/mises-en-pratique/standard-frequencies-second).
No new transition has been proposed therefore the list of 14 transitions is unchanged from 2017 and the conventional numbering is retained:

nu1 $^{115}In^+$
nu2 ^{1}H
nu3 ^{199}Hg
nu4 $^{27}Al^+$
nu5 $^{199}Hg^+$
nu6 $^{171}Yb^+$(E2)
nu7 $^{171}Yb^+$(E3)
nu8 ^{171}Yb
nu9 ^{40}Ca
nu10 $^{88}Sr^+$
nu11 ^{88}Sr
nu12 ^{87}Sr
nu13 $^{40}Ca^+$
nu14 ^{87}Rb

Measurements are associated either with one value nuI in the case of absolute measurement with respect to the SI second, or with two values nuI and nuJ in the case of measurements of a ratio nuI / nuJ. The conventional identification of measurements is qX where X is an index varying from 1 to the total number of measurements (106 in the 2021 adjustment).

The WGFS decided to include correlations between the different measurements as much as possible, so that the formal uncertainties obtained from the adjustment may be considered as realistic as possible. This memo describes the computation of correlations between absolute measurements due to using the same PFS or SFS to access the SI second. For completeness it also includes the list of the other correlations coefficients which were independently computed and took into account other sources of correlations.

1. Principle of computation of correlations

1.1 General formulation

This is described in a paper developed for the ROCIT project [1].

1.2 Correlation due to the access to the SI second

We want to estimate the correlation between absolute frequency measurements due to using the same PSFS to access the SI second, either directly or through d_{TAI}. The formula to be used is written as

$$\mathrm{Coef}(1,2) = \left[\sum_{i,j} w_i w_j \sum_k \left(w_{i,k} u_{BS_{i,k}} w_{j,k} u_{BS_{j,k}} \right) \right] / u_{Tot_1} \times u_{Tot_2} \quad (1)$$

where

i indexes the months used to access the SI second for measurement 1 and w_i is the weight of month i in accessing the SI second for measurement 1 : $\Sigma_i w_i = 1$
j is the index of months for measurement 2: $\Sigma_j w_j = 1$
k is the index of PSFS and $w_{i,k}$ is the weight of PSFS k in the estimation of d for month i: $\Sigma_k w_{i,k} = 1$; $\Sigma_k w_{j,k} = 1$; $0 \leq \Sigma_k w_{i,k} wj_{,k} \leq 1$
u_{Tot} is the total uncertainty of the measurement 1/2.
$u_{BSi,k}$ is the stationary part of u_B for PSFS k in month i, i.e. the part of u_B that correlates measurements of the same standard at different periods. It is noted u_{Bsta} below.

Formula (1) is explicitly written for the case of measurements which access the SI second through d_{TAI} over several months. However it can be used as well for measurements which access the SI second through specific PSFS by adapting the summation on index k to the problem at hand. However it should be kept in mind that, in that case, the correlation through the access to the SI second may not be the dominant part of the correlation between the two measurements. This is particularly the case for measurements which access the SI second through local PSFS, and all the more when the two measurements are carried out in the same laboratory. Nevertheless, for the 2021 adjustment, formula (1) has been used to compute the correlation between two measurements with access to the SI second through local PFS when no better estimation of the correlation was available.

2. Implementation

All programs and data files, input and output of the computation can be accessed in the repository (TO BE COMPLETED).

2.1 Determination of the PSFS contributions to the BIPM monthly d_{TAI} values

In the web page https://webtai.bipm.org/ftp/pub/tai/other-products/etoile/ can be found the files ETyy.mm which contain, for each month mm (from 01 to 12) of year 20yy, the list of the PFS and SFS evaluations that were used to compute the d_{TAI} value for that month and, under the heading 'Coef.', the weight (normalized to unity) of each evaluation in the estimation of d_{TAI} as well as the standard uncertainty u_B for each evaluation. An example follows:

```
                 Measurements                   in 10**-13
  Code    Standard Start    End  f(EAL)-f(st.) Uncert.A Uncert.B    Coef.     Residual Norm.Res
 1920502 PTB CSF2 59179. 59204.    6.50561  0.00159   0.00170    0.158753  0.00268   1.15326
```

From these files a program `read_et.f` generates a new file which lists, over a specified period, the total weight of each PFS or SFS in the estimation of d_{TAI} and the value of u_B for each standard. For our analysis the period 01/2014 to 10/2020 has been chosen to cover nearly all recent accurate measurements of OFS which used d_{TAI} as an access to the SI second and for other practical reasons (change of format in ET files in 01/2014, estimation of u_{Bsta} for the PFS, see section 2.2).
An excerpt of the output file follows, where we see that in the month 10/2018, the estimated d_{TAI} had an uncertainty $1.95\text{x}10^{-16}$ and e.g. PTB-CsF2 had a weight of 39.4% with an u_B value of $2.0\text{x}10^{-16}$. Note that standards which contributed with weights lower than 0.05% are not indicated.

```
              PTB CSF1PTB CSF2OP  FO1 OP  FO2 OP  FOM IT  CsF2NPL CsF2SU  FO2 NIM NIM5OP  FORb
               1920501 1920502 1920802 1920803 1920804 1921102 1921702 1923802 1924801 1930803
201810   1.950     2.91    39.40    20.30    28.51             0.08             0.33            8.39
                   3.21     2.00     3.22     2.01             1.70             2.40     9.00   6.50
```

Two such files are generated,
`readet.out_ubtot` in which the full u_B value of each PFS/SFS is indicated
`readet.out_ubcor` in which an estimation of the stationary part of u_B, here noted u_{Bsta}, is provided for some PFS (see section 2.2). This file was used in the computation of correlations for the final adjustment.

2.2 Determination of the component u_{Bsta} for the different PSFS

In principle, only the part of the u_B uncertainty of PSFS that is correlated from month to month should be used in equation (1), however a specific analysis is required to determine this value for each PSFS and there is some ambiguity in determining which part of the uncertainty is correlated and which part is independent between successive evaluations of a PSFS. Because five PSFS (PTB-CsF1 and CsF2, SYRTE-FO1, FO2 and FO2(Rb) make, on average, more than 90% of the monthly estimation of d_{TAI} over the period we are interested in, a specific analysis has been carried out for them. See in Annex 1 the u_{Bsta} values determined for the LNE-SYRTE and PTB fountains. For all other PSFS, the full u_B value has been used in applying equation (1).

2.3 Computation of the correlation coefficients

Two input files are necessary:

- From the file of the measurements in the usual format is created an "extended" input file, here named `InputData_full_YYYYMMDD` where `YYYYMMDD` is the date of run, which includes the information on the access to the SI second. See some examples providing the format to express the additional information in Annex 2.
- The file `readet.out_ubtot` or `readet.out_ubcor` as described in section 2.1.

From these files a program `calc_cor.f` generates a file `calc_cor.res_YYYYMMDD_ubxxx` containing the list of coefficients in the required format.

3. Correlation results used for the 2021 adjustment

3.1 Input data for the main runs

We have 70 « absolute frequency » measurements (not counting 3 that have been deweighted). In this analysis, we computed correlations due to the access to the SI second between 34 of them, as follows:

- 33 which period of measurement is not older than 2014
- 1 earlier measurement (q46, nu12, i.e. 87Sr from [LeTargat2013]) because it has a small uncertainty and significant correlation with more recent measurements.

In total 12 concern ^{87}Sr, 6 for ^{171}Yb, 3 for ^{171}Yb^{+}(E3) and ^{40}Ca^{+}, 2 for ^{115}In^{+}, ^{88}Sr and ^{87}Rb, and one for ^{199}Hg, ^{27}Al^{+}, ^{171}Yb^{+}(E2) and ^{88}Sr^{+}.

The access to the SI second was modelled as follows, depending on the method of access:

- In case of access through d_{TAI} (20 measurements), by specifying the list of months along with the weight they got in the determination. In the simplest case, there is only one month used and it has weight 1.00.
- In case of access through individual PSFSs (14 measurements), by assigning the ensemble of individual comparisons to a set of months and estimating for each month a weight based on the information available in the published reference (typically a plot of residuals indicating dates and uncertainties). For each month, the weight is then shared between the PSFS used during that month.

See Annex 3 for some detail on the list and on the information on the access to the SI second.

Runs with 34 absolute measurements provided 561 correlation coefficients for possible use in the adjustment: 190 between measurements using d_{TAI} as access to the SI second, 280 between one measurement using d_{TAI} and one measurement using PSFSs, and 91 between measurements using PSFS (for which our determination may miss other significant sources of correlation). The run with the file `readet.out_ubtot` provides the set of coefficients below named Cor_{tot}, the run with the file `readet.out_ubcor` provides the Cor_{sta} set of coefficients.

3.2 Comparison to Marco Pizzocaro results

A set of 888 correlation coefficients between 73 measurements of the list (56 absolute and 17 ratios) was provided by Marco Pizzocaro [2]. The intersection of Marco's list with our set of 561 coefficients contains 204 coefficients, all between pairs of absolute frequency measurements, including 78 between measurements using d_{TAI} as access to the SI second. For those 78 coefficients, the agreement between our set Cor_{tot} and Marco's set is quite good: a mean difference of 0.005 with a standard deviation of 0.008. Because Marco's computation used the full u_B value to estimate correlations, the comparison to Cor_{tot} is adequate.

3.3 The chosen set of correlations

3.3.1 Modification to the input data

The WGFS decided to modify the uncertainties of q1 (x3), q31 (x1.5), q51 (x100), q52 (x6), q74 and q78 (x3), q88 and q105 (x2). This is reflected in the computation of coefficients for q74, q88 and q105.
Following the initial computation of correlation coefficients, it was found unrealistically large values for q73 and q98. After analysis, it was determined that both measurements, which used PTB-CsF1 and CsF2 as access to the SI second, considered the PFS u_B values to be much less correlated than was assumed in our analysis. As the individual measurements were provided in the publications, a new determination of the measurements' uncertainties was carried out using our hypothesis for u_B correlation. This resulted in the q73 uncertainty expanded from 1.5×10^{-16} to 1.65×10^{-16} and the q98 uncertainty expanded from 1.3×10^{-16} to 1.6×10^{-16}.

3.3.2 Final set

The final expanded input file is `InputData_full_20210317`. The final set of coefficients from this analysis (file `calc_cor.res_20210317_ubcor`) includes 399 values > 0.001, of which 56 are larger than 0.1.
396 were used in the adjustment of reference frequencies, those not included are

```
r(q14,q18)     0.131
r(q46,q47)     0.324
r(q50,q90)     0.037
```

In addition 87 coefficients were computed in a series of different analyses. The list is in Annex 4.
The total number of correlation coefficients was then 483.

References

[1] Margolis H., Pizzocaro M., Guidelines on the evaluation and reporting of correlation coefficients between frequency ratio measurements, 18SIB05 ROCIT Document, 25 July 2020.
[2] Pizzocaro M. Correlations in the measurements of optical clocks, 14 April 2020, personal communication

Annex 1: More details on the computation of u_{Bsta} for LNE-SYRTE and PTB standards

A specific estimation of u_{Bsta} was attempted for the PFS/SFS which have the highest weight in d_{TAI}, i.e. those which have the most evaluations and low uncertainty. This concerns mostly the fountains FI1, FO2 and FO2(Rb) from SYRTE and the fountains CSF1 and CSF2 from PTB.

LNE-SYRTE fountains:
Following exchanges with Michel Abgrall and Luca Lorini, it was considered that, among the main components of u_{Bsta}, those relative to the Zeeman, Blackbody and MW lensing shifts were about constant but two other components had significant variations over the years:
1. the collisional shift uncertainty, estimated as a given fraction of the value of the collisional shift. The collisional shift itself is varies at each evaluation, however it was possible to identify large periods of time over which the shift value and the fractional value providing the uncertainty were considered constant for each fountain (i.e. there were no variations by more than 50% from the chosen value).
2. the gravitational shift uncertainty; the value and uncertainty of the shift was changed for the three fountains for the data of March 2018.
It was also determined that this computation of u_{Bsta} was not necessary for SYRTE-FOM which has a higher uncertainty and fewer evaluations.
The resulting values of u_{Bsta} may be found below for the three fountains.

SYRTE-FO1 (3 periods):
201401 to 201802: 2.5×10^{-16} (2.0 for u_{Coll}, 1.0 for u_{Grav})
201803 to 201808: 2.3×10^{-16} (2.0 for u_{Coll}, 0.25 for u_{Grav})
201809 to 202012: 1.7×10^{-16} (1.3 for u_{Coll}, 0.25 for u_{Grav})

SYRTE-FO2 (3 periods):
201401 to 201509: 1.8×10^{-16} (1.2 for u_{Coll}, 1.0 for u_{Grav})
201510 to 201802: 1.5×10^{-16} (0.2 for u_{Coll}, 1.0 for u_{Grav})
201803 to 202012: 1.2×10^{-16} (0.4 for u_{Coll}, 0.25 for u_{Grav})

SYRTE-FO2(Rb) (3 periods):
201401 to 201509: 2.3×10^{-16} (1.2 for u_{Coll}, 1.0 for u_{Grav})
201510 to 201802: 2.1×10^{-16} (0.6 for u_{Coll}, 1.0 for u_{Grav})
201803 to 202012: 1.8×10^{-16} (0.2 for u_{Coll}, 0.25 for u_{Grav})
The uncertainty u_{Srep} is also taken into account in computing the final correlated part of the uncertainty.

PTB fountains:
Stefan Weyers provided a table of estimated values of u_{Bsta} for all individual fountain evaluations. As for the SYRTE fountains, it was possible to identify large periods of time over which the values u_{Bsta} were considered constant for each fountain. The resulting values of u_{Bsta} may be found below for the two fountains.

PTB-CsF1
201401 to 201902: 3.1×10^{-16} ; (1)
201903 to 202012: 2.0×10^{-16} ;
(1) Over the period 201401 to 201603, the u_B uncertainty stated for PTB-CsF1 in the TAI reports was of order 7×10^{-16}. It was later determined that an u_B value of order 3×10^{-16} is more realistic. The u_{Bsta} has been estimated based on the a posteriori realistic approach. Because the original (large) u_B values have been used when d_{TAI} was calculated, this will result in somewhat underestimated correlations coefficients.

PTB-CsF2
201401 to 201802: 2.5×10^{-16} ;
201803 to 201808: 2.3×10^{-16} ;
201809 to 202012: 1.7×10^{-16} ;

Annex 2: Sample input file with model of the access to the SI second

The usual input file is expanded for each measurement with the information on the access to SI second, with one line per month including:
Weight of the month (from 0.001 to 1.000)
Designation of the month `YYYYMM`
In case of access through d_{TAI}, the first line includes an identification of the laboratory.
In case of access through PSFS, each monthly line contains a series of pairs (PSFS name, PSFS weight) used in this month with the sum of the weights per month equal to 1.000.

Example with access through d_{TAI} over four months, each month with equal weight.

```
q55     nu13           411042129776401.7     1.1     [Huang2015,2014/15value] ! Weights TO BE CHECKED
0.250  201411  WUHA
0.250  201412
0.250  201501
0.250  201502
```

Example with access through PSFS over four months, each month with equal weight. Two or three PSFS per month.

```
q47     nu12           429228004229872.92    0.12    [Lodewyck2016]          ! Weights TO BE CHECKED
0.250  201409  OP-FO1    0.250  OP-FO2    0.400  OP-FOM    0.350
0.250  201410  OP-FO2    0.600  OP-FOM    0.400
0.250  201503  OP-FO2    0.600  OP-FOM    0.400
0.250  201506  OP-FO1    0.250  OP-FO2    0.400  OP-FOM    0.350
```

Annex 3: List of absolute measurements for computing correlation

The table below lists the 34 absolute measurements between which correlations due to the access to the SI second have been computed. The information in the last three columns has been manually added:

- LABO indicates the laboratory where the standard was operated. The purpose is to point those correlations between standards operated in the same lab so as to take care of them separately.
- #months indicates the number of UTC months over which the comparison to the SI second took place. The detailed list is in the complete input file.
- #PSFS indicates the number of PFS or SFS which were used to access the SI second. 0 means access through d_{TAI}. The detailed list is in the complete input file.

#	q-value	Trans.	LABO	#months	#PSFS
1	3	nu1	NICT	2	0
2	7	nu3	OP	2	1
3	14	nu6	NPL	2	1
4	18	nu7	NPL	2	1
5	24	nu8	IT	4	1
6	25	nu8	KRIS	1	0
7	32	nu10	NRC	2	0
8	34	nu11	POL	1	0
9	35	nu11	POL	1	0
10	43	nu12	NMIJ	1	0
11	44	nu12	NIM	2	1
12	46	nu12	OP	1	3
13	47	nu12	OP	4	3
14	48	nu12	PTB	1	1
15	49	nu12	PTB	1	2
16	50	nu12	NICT	3	0
17	55	nu13	WUHA	4	0
18	56	nu14	OP	37	0
19	58	nu14	OP	1	4
20	70	nu8	ECNU	1	0
21	71	nu7	NPL	1	0
22	72	nu12	NPL	1	0
23	73	nu12	PTB	10	1
24	74	nu1	NICT	1	0
25	75	nu8	NIST	8	0
26	76	nu8	IT	5	0
27	88	nu13	WUHA	1	0
28	89	nu8	NMIJ	6	0
29	90	nu12	NICT	14	0
30	91	nu12	IT	2	1
31	96	nu12	NIST	4	0
32	97	nu4	NIST	5	0
33	98	nu7	PTB	10	2
34	105	nu13	NIM	1	1

Special cases:

- q46 (^{87}Sr Le Targat 2013): The measurement dates from 2011, but it is declared as 01/2014 in the input file in order to allow its treatment. SYRTE fountains are assumed to be equivalent in 2011 and 2014 for the purpose of computing correlations.
- q56: (^{87}Rb SYRTE data) Measurements are from Jan 2012 to April 2017 but only 37 months after 01/2014 appear in the input file. More weight (5% vs. 2.5%) was given to the first three months to account for measurements before 2014.
- q90 (^{87}Sr Nemitz 2020): Actually used 63 PFS reports to TAI covering 14 months from 04/2016 to 03/2020. Because the PFS reports were chosen based on their high weight in the determination of d_{TAI}, we considered that it would be equivalent, and simpler, to model the access to TAI as if it was through 14 monthly d_{TAI} values.
- q73 (^{87}Sr Schwartz 2020) and q98 ($^{171}Yb^{+}$(E3) Lange 2021): The measurements vs. PTB fountains provided on dense figures are synthetized as 10 monthly values with equivalent weight (10% each).
- q7, q14, q18, q44, q47, q50, q55, q89, q91: Weights were split equivalently over the given number of months.

In all other cases where #months > 1: Weights for each month were either directly given in the publication, or provided by personal communication or determined by analysis of figures and tables in the publication.

Annex 4: List of additional correlation coefficients

r(q14,q18)	0.680
r(q14,q63)	0.507
r(q18,q63)	-0.018
r(q19,q45)	0.981
r(q46,q47)	0.324
r(q73,q92)	-0.060
r(q92,q98)	0.002
r(q92,q99)	-0.009
r(q98,q99)	-0.002
r(q13,q14)	0.030
r(q13,q63)	0.060
r(q16,q18)	0.004
r(q16,q63)	-0.007
r(q18,q19)	0.009
r(q19,q63)	-0.015
r(q16,q19)	0.006
r(q81,q91)	-0.123
r(q7,q60)	0.449
r(q7,q61)	0.221
r(q47,q60)	-0.033
r(q47,q69)	0.018
r(q47,q84)	-0.018
r(q47,q85)	-0.022
r(q47,q100)	-0.026
r(q47,q101)	-0.022
r(q49,q86)	-0.004
r(q49,q87)	-0.007
r(q58,q61)	-0.636
r(q58,q69)	-0.713
r(q60,q61)	0.456
r(q60,q69)	-0.028
r(q60,q84)	0.028
r(q60,q85)	0.035
r(q60,q100)	0.041
r(q60,q101)	0.035
r(q61,q69)	0.597
r(q69,q84)	-0.015
r(q69,q85)	-0.019
r(q69,q100)	-0.022
r(q69,q101)	-0.019
r(q71,q84)	0.092
r(q71,q85)	0.112
r(q71,q86)	0.086
r(q71,q87)	0.151

r(q84,q85)	0.155
r(q84,q86)	0.105
r(q84,q87)	0.183
r(q84,q100)	0.117
r(q84,q101)	0.100
r(q85,q86)	0.128
r(q85,q87)	0.224
r(q85,q100)	0.027
r(q85,q101)	0.023
r(q86,q87)	0.178
r(q100,q101)	0.027
r(q31,q57)	0.165
r(q53,q68)	-0.672
r(q56,q106)	-0.277
r(q58,q106)	-0.392
r(q61,q106)	0.329
r(q69,q106)	0.369
r(q95,q106)	0.221
r(q24,q81)	0.088
r(q76,q82)	0.191
r(q76,q83)	0.175
r(q82,q83)	0.386
r(q3,q78)	0.028
r(q3,q74)	0.026
r(q41,q90)	0.001
r(q50,q90)	0.061
r(q59,q79)	0.826
r(q66,q79)	-0.009
r(q74,q78)	0.859
r(q78,q80)	0.006
r(q78,q90)	-0.021
r(q78,q94)	0.005
r(q80,q90)	-0.026
r(q89,q93)	0.748
r(q89,q94)	0.672
r(q89,q95)	0.860
r(q90,q94)	-0.033
r(q93,q94)	0.603
r(q93,q95)	0.680
r(q94,q95)	0.611
r(q102,q103)	0.615
r(q102,q104)	-0.207
r(q103,q104)	0.329