Absolute frequency of $^{87}\text{Sr}$ at $1.8 \times 10^{-16}$ uncertainty by reference to remote primary frequency standards

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Abstract
The optical lattice clock NICT-Sr1 regularly reports calibration measurements of the international timescale TAI. By comparing measurement results to the reports of eight primary frequency standards, we find the absolute frequency of the $^{87}\text{Sr}$ clock transition to be $f(\text{Sr}) = 429 228 004 229 873.082 \, \text{Hz}$, with a fractional uncertainty of less than $1.8 \times 10^{-16}$ approaching the systematic limits of the best realization of the SI second. Our result is consistent with other recent measurements and further supported by the loop closure over the absolute frequencies of $^{87}\text{Sr}$, $^{171}\text{Yb}$ and direct optical measurements of their ratio.

Keywords: atomic clock, frequency standard, SI second, strontium, optical clock, lattice clock

1. Introduction
Optical clocks, frequency standards that probe atomic references in the optical frequency regime, now reach uncertainties close to one part in $10^{18}$, enabling new science such as relativistic geodesy, dark matter searches and investigations of changes in fundamental constants [1–6]. Yet, all of our daily interaction with International Atomic Time (TAI) and its derived timescales rely on continuity above all else. To ensure this, the consultative committee for time and frequency (CCTF), instituted by the comité international des poids et mesures (CIPM), has defined a set of milestones [7] to be reached before the definition of the SI second will change from the currently referenced microwave transition in caesium ($^{133}\text{Cs}$) to an optical reference with significantly greater accuracy.

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One of these milestones is contribution of optical clocks to the steering of TAI according to the procedures established for $^{87}\text{Rb}$ microwave standards [8]. Following pioneering work at LNE-SYRTE [9], our own NICT-Sr1 and several other optical lattice clocks [10, 11], have been officially recognized as secondary frequency standards (SFS). After recognition in November 2018, NICT-Sr1 has contributed to the steering of TAI by reporting measurement results for inclusion in the monthly circular T issued by the International Bureau of Weights and Measures (BIPM). As a clock utilizing the $^1S_0 \rightarrow ^3P_0$ transition in neutral $^{87}\text{Sr}$, the weight of these contributions is now limited by an uncertainty of $4 \times 10^{-16}$ this transition has been assigned as a secondary representation of the second (SRS) [7] based on previous measurements (references [9, 12–15] among others) of the absolute frequency.

Here we present a new evaluation of the Sr absolute frequency, referencing the ensemble of caesium-based primary frequency standards (FPS) that submit TAI evaluations to BIPM. The results are consistent with the latest published results [16] for a comparison to local standards. Our evaluation not only tests the performance of the clocks, but in employing the same infrastructure used in the steering of TAI, it directly
Figure 1. Remote comparison of NICT-Sr1 to international timescales for absolute frequency evaluation. ① The optical lattice clock NICT-Sr1 characterizes the frequency of a HM. ② This HM is also continuously compared to NICT’s local timescale UTC(NICT) within the JST system. ③ The BIPM evaluates submitted data of GNSS to find the time deviation of UTC(NICT) from the calculated UTC scale. The evolution of this deviation provides the frequency difference. Combining ①–③ characterizes the frequency of UTC (and the identical frequency of TAI) through measurements of NICT-Sr1, typically expressed as the deviation of the TAI scale interval $d$. Calculated for each frequency standard reporting to BIPM, the collective estimates of the deviation are used to steer TAI. We use the same values to compare the frequency of NICT-Sr1 to remote frequency standards operated by institutes worldwide.

supports a greatly reduced SRS uncertainty of $1.8 \times 10^{-16}$ or below.

2. Methods

Over four years of operating NICT-Sr1, we have accumulated 776 h of data with a well-characterized link to TAI, suitable for determining the absolute frequency of the $^{87}$Sr clock transition. An evaluation of the current frequency deviation of TAI is conveniently available in the circular T, but relying on this monthly value often incurs additional uncertainty, particularly when the results for the clock under evaluation and for the remote references both require extrapolation to the full reporting period. On request, BIPM can provide a frequency evaluation with a finer 5 days resolution to mitigate this problem [17]. However, this evaluation includes the results of any contributing secondary standard, which is undesirable in an absolute frequency measurement that seeks to reference the SI second as defined. Here, the results after 2018 would also contain contributions from NICT-Sr1 itself.

Sections 2.1–2.10 describe a new method that directly traces measurements by NICT-Sr1 to individual primary frequency references, using the international timescale only as a flywheel oscillator. This allows for arbitrary evaluation periods with the same 5 days resolution and is based on information made publicly available by BIPM. Tracing measurements over 13 periods of estimation to 8 primary caesium fountain standards provides a total of 63 datapoints, which are then combined to find the absolute frequency. Sections 2.11 and 2.12 describe statistical methods to obtain weights and uncertainties in the presence of multiple sources of correlated errors.

Figure 1 gives a schematic overview of tracing the frequency of the optical clock NICT-Sr1 to the international timescales. The clock is operated intermittently [18], with

Table 1. Nominal uncertainty budget of NICT-Sr1.

| Effect                              | Correction ($10^{-17}$) | Uncertainty ($10^{-17}$) |
|------------------------------------|-------------------------|--------------------------|
| Blackbody radiation                | 513.9                   | 3.0                      |
| Light shifts                       | 2.6                     | 3.8                      |
| DC Stark shift                     | 0.1                     | 0.5                      |
| Quadratic Zeeman shift             | 52.0                    | 0.3                      |
| Hot and cold collisions            | 2.2                     | 2.3                      |
| Servo error                        | 0.0                     | 0.6                      |
| Total                              | 570.8                   | 5.4                      |
| Gravitational redshift             | –834.1                  | 2.2                      |
| Total (with redshift)              | –263.3                  | 5.9                      |

NICT’s ensemble of hydrogen masers (HMs) bridging measurement gaps to obtain the continuous interval needed for an accurate satellite link. The Échelle Atomique Libre (EAL) underlyng TAI then similarly provides the stability to extrapolate to the reporting intervals of different reference standards.

2.1. Optical clock

The optical lattice clock NICT-Sr1 typically traps 1000 $^{87}$Sr atoms in a vertical, one-dimensional optical lattice created by the standing wave of a laser tuned to a magic wavelength near 813 nm, where it provides tight confinement with negligible disturbance to the atomic resonance frequency [19]. By detecting the excitation state of the trapped atoms, a clock laser is then stabilized to the transition frequency of approximately 429 228 004 229 873 Hz. Measurements destroy the atomic sample, limiting the clock to periodic evaluations with a cycle time of typically 1.5 s. A reference cavity made of ultra-low-expansion glass thus serves as a flywheel oscillator. With atomic measurements providing corrections for changes in the cavity’s resonant frequency and drift rate, the clock laser
realizes a continuous optical reference with a frequency-noise limited fractional instability that falls with averaging time $\tau$ as $\sigma_f(\tau) = 7 \times 10^{-15} (\tau/\text{s})^{-1/2}$. The systematic uncertainty evaluation of NICT-Sr1 is described in reference [15]. Table 1 shows the nominal uncertainty budget with an overall fractional uncertainty $\sigma_0 = 5.4 \times 10^{-17}$, largely limited by the evaluation of residual lattice light shifts. Each measurement submitted to BIPM is accompanied by a report that includes a specific uncertainty budget [20].

The servo error uncertainty represents the possibility of a persistent deviation of the clock laser frequency from the atomic resonance, as may occur due to incomplete cancelation of the cavity drift. The mean deviation observed in data accumulated over the four years is $3.7 (4.6) \times 10^{-18}$. We thus reassign a conservative uncertainty of $\sqrt{0.37^2 + 0.46^2} \times 10^{-17} = 0.59 \times 10^{-17}$. This represents errors that affect all measurements equally, while random instabilities are handled as part of the statistical contribution.

### 2.2. Intermittent clock operation

International timescale comparisons rely on satellite links, either by two-way satellite time-and-frequency transfer or by precise point positioning over global navigation satellite systems (GNSS), as used at NICT. The accuracy of these links relies on long uninterrupted measurements, modelled by an atomic maser, as used at NICT. The accuracy of these links for short interruptions in clock operation, but also for intervals of multiple days. This opens the path to intermittent clock operation NICT-Sr1 in a pattern of intermittent measurements [18, 26] and use the flywheel HM to extend the effective period of evaluation. Similar approaches have also been adopted in other optical clock measurements that rely on remote links [10, 11, 16, 27].

### 2.3. Evaluation of reference maser frequency

During the operation of NICT-Sr1, an optical frequency comb compares the optical reference to the signal of the reference HM at $f_{HM} = 100$ MHz. All measurements are performed phase-coherently without deadtime to provide efficient suppression of phase noise in the HM signal. For averaging times $\tau > 10$ s, the observed instability approximately follows $\sigma_f(\tau) = 4 \times 10^{-14} (\tau/\text{s})^{-1/2}$ until the drift of the HM frequency limits the stability. The drift rate is very consistent [28], and the instability of drift-removed data matches the expected flicker noise floor. Section 2.7 discusses the observed HM instability in more detail.

To minimize measurement noise and avoid counting errors, the frequency comb measurements are performed as illustrated in figure 1. The HM signal is multiplied by a factor $m$ using a phase-locked dielectric resonator oscillator (PLDRO, Nexyn Corporation NXPLOS). The $n$th harmonic of the comb repetition rate $f_c$ is detected by a high-speed photodetector (Discovery Semiconductors DSC40S) at the output of the same amplified and frequency-broadened optical path that is used to generate the beat signal with the clock laser. By downmixing this signal with the output of the PLDRO, the counted frequency (indicated by $\delta$ in figure 1) becomes

$$f_c = nf_i - mf_{HM} = 50 \text{ MHz}$$

for a typical configuration with $m = 92$, $n = 37$ and $f_i = 250$ MHz. This relaxes the requirements on the counter accuracy by a factor of $(nf_i)/f_c = 185$. Detector and PLDRO operate in a temperature-stable environment and protected from air currents. A zero-deadtime multichannel counter (K&K Messtechnik FXE) measures $f_c$ simultaneously with the clock laser’s beat $f_b$ with the nearest comb line $f_{clk}$ and the comb’s carrier-envelope offset $f_{CEO}$, obtained from an $f - 2f$ interferometer. The clock laser frequency, as it appears at the comb, can then be determined as

$$f_{clk} = f_{CEO} + f_{clk}f_i + f_b$$

(2)

The measurements of $f_{CEO}$ and $f_b$ are also used to detect disturbances of the clock laser frequency and cycle slips of the comb lock, so that affected data can be removed from the evaluation. When the comb is locked to the clock laser, the small in-loop error of $f_b$ allows direct detection of even single-cycle slips over the 1 s measurement interval. When the comb is locked to the HM for greater robustness, we operate an additional tracking oscillator that is phase-locked to the $f_b$ signal with narrow control bandwidth. Counted as $f_c$ on a separate counter channel, laser disturbances will then cause different-valued miscounts and yield $|f_i - f_b| > 1$ Hz. This allows unreliable data to be rejected despite a noise band of $f_b$ that is wider than 1 Hz.

The primary concern in terms of systematic measurement errors are then phase shifts induced by thermal effects on the cables delivering the HM signal from the adjacent building that is home to the JST system. Presuming a daily temperature cycle, this may lead to persistent errors if measurements typically occur at the same time of day. We test for these effects
in the data set of a nearly continuous ten-day measurement by binning the data by time-of-day and examine a sliding six-hour window to obtain maximum sensitivity to diurnal effects. We observe no excursions beyond statistical expectations. For the specific time window of 14:00 to 20:00, where most measurements are performed, we set a limit of \( u_d = 7.95 \times 10^{-17} \) by adding the observed deviation from the mean in quadrature with the statistical uncertainty and then take \( u_{\text{b}/\text{lab}} = u_d \) as the systematic uncertainty for the frequency link to the reference HM. For longer measurement intervals, cyclical phase shifts will have less effect, and we model this as a systematic uncertainty falling as \( u_{\text{b}/\text{lab}} = u_d (T_i/6\text{h}) \) for measurements with individual operating times \( T_i > 6\text{h} \).

Measurements before MJD 58 400 acquired a lower (1 GHz) harmonic of the repetition rate directly from the comb oscillator, which was then frequency divided to 100 MHz for phase comparison to the HM reference. These measurements showed sensitivity to the thermal environment of the frequency divider. Additionally, the phase comparator was found to introduce a persistent error depending on the measured fractional frequency difference \( \Delta y \approx 10^{-12} \) as \( \delta_{\text{pc}} = 4.6 \times 10^{-5} \Delta y \). This results from numerical errors in the original software version and a frequency error of the integrated timebase. After an initial thermalization for 12 h, a test at \( \Delta y \approx 0 \) finds counter and phase comparator measurements to agree to \( \delta y = 6.6 \times 10^{-19} \) over 48 h.

Measurements relying on phase comparator data accommodate this by a larger systematic uncertainty \( u_{\text{b}/\text{lab}} = 1.0 \times 10^{-16} \). As summarized in table 3, we now apply a retroactive correction for \( \delta_{\text{pc}} \) based on our present understanding, but maintain the originally reported uncertainty as \( u_{\text{b}/\text{lab}} = u_d + u_{\text{pc}} \). The phase comparator errors represented by \( u_{\text{pc}} = 6.1 \times 10^{-17} \) are taken to be correlated across all affected measurements, but statistically independent from the diurnal effects.

### 2.4. HM drift correction

We consider the observed HM fractional deviation \( y_{\text{obs} }^{\text{HM}} (t) \) from the nominal frequency to consist of a constant linear drift \( y_{\text{lin} }^{\text{HM}} (t) \) with superimposed noise of zero mean value. We seek the mean value \( y_{\text{HM}} \) over the chosen evaluation period \( T \). As illustrated in figure 2, we approach the drift by fitting the observed subset data as

\[
y_{\text{lin} }^{\text{HM}} (t) = y_{\text{obs} }^{\text{HM}} + a (t - \bar{t}) ,
\]

where the observed mean value \( y_{\text{obs} }^{\text{HM}} \) corresponds to the value at the barycentre \( \bar{t} \). Performing the fit relative to this point, which represents the mean of all observation times, provides the clearest separation of the uncertainties of the observed mean value and of the drift rate.

Analysis (see section 2.5) finds the instability at the original 1 s measurement interval to be dominated by phase noise. We bin the frequency data over 10 s intervals where this is suppressed to below the level of white frequency noise (WFN). The fit to the binned data can then be interpreted in the context of normally distributed, uncorrelated noise. Finding \( y_{\text{HM}} \) from \( y_{\text{obs} }^{\text{HM}} \) now requires a correction from the barycentre \( \bar{t} \) to the midpoint \( t_M \) of the evaluation period

\[
\delta y_{\text{mid}} = a (t_M - \bar{t}) \approx y_{\text{HM}} - y_{\text{obs} }^{\text{HM}}
\]

that carries an uncertainty \( u_{\text{mid}} = \sigma_a |t_M - \bar{t}| \), where the slope \( a \) and its uncertainty \( \sigma_a \) are obtained from the fit. The statistical uncertainty \( u_{\text{stat}} \) of \( y_{\text{obs} }^{\text{HM}} \) is evaluated separately as below.

### 2.5. Short-term measurement instability

After subtracting the fitted linear drift, the Allan deviation of the residuals provides information on the instabilities of the HM and the measurement of its frequency. At short averaging times, where phase noise of the HM signal strongly contributes to the instability, the reference cavity serves as a stable flywheel oscillator, and in conjunction with the zero-deadtime frequency measurement avoids the aliasing effects [29] that typically accompany cyclic clock interrogation. The instability initially falls as approximately \( \sigma_y (\tau) \propto \tau^{-1} \), before the slope follows \( \sigma_y^{\text{WFN}} (\tau) \propto \tau^{-1/2} \) over averaging times 10 s < \( \tau < 10^4 \) s, consistent with WFN as the primary noise process. We extrapolate this trend to the total measurement time \( T_i \) for the evaluation period to find \( u_{\text{stat}} = \sigma_y^{\text{WFN}} (T_i) \). Figure 3 illustrates the observed instability, where we find \( u_{\text{stat}} = 3.9 \times 10^{-17} \) for \( T_i = 779853 \) s of exemplary data acquired over ten days of near-continuous clock operation.
2.6. Long-term HM instability

The excess instability observed at long averaging time represents stochastic HM behaviour that we seek to quantify. It does not limit the accuracy of the measured mean frequency. However, similar behaviour during unobserved intervals leads to a deadtime uncertainty. As discussed in reference [14], extrapolating the frequency of a flywheel oscillator—characterized by a known noise power spectral density (PSD) $S_N$—from one distribution of measurements to another incurs an uncertainty according to

$$u_{\text{loc}}^2 = \int_0^\infty S_N(f) |G_\Delta(f)|^2 \, df.$$  (5)

Here $G_\Delta(f)$ is the Fourier transform of the differential weighting function $g_\Delta(t) = g_1(t) - g_2(t)$, where normalized functions $g_1(t)$ and $g_2(t)$ describe the two distributions, in this case representing observation intervals and the full evaluation period.

We handle phase and white frequency noise as part of $u_{\text{stat}}$ to better account for excess noise in the measurement system or varying day-to-day performance. Long-term HM behaviour under the operating conditions at NICT is described by a model Hadamard variance

$$\sigma_H^2(\tau) = (2.1 \times 10^{-16})^2 + (1.7 \times 10^{-17} \tau/1\text{d})^2$$  (6)

that accounts for FFN and FWFM. A corresponding PSD can then be calculated [30] from the sensitivity function of the Hadamard deviation [24] as

$$S_N^{\text{HM}}(f) = 4.0 \times 10^{-32} \, (f/\text{Hz})^{-1}$$

$$+ 3.0 \times 10^{-45} \, (f/\text{Hz})^{-3}.$$  (7)
The requirements are given in Table 2. In the presence of the steep slope of $S_1(f)$ near $f = 0$ Hz, zero-padding the differential weight $g_{\Delta} \, (t)$ improves the accuracy of the calculations when using a discrete Fourier transform to obtain $G_{\Delta} \, (f)$. We find the results in good agreement with a Monte Carlo analysis using random noise specified by $S_1(f)$ according to reference [31].

Early measurements used a less flexible stochastic model [15, 18]. Although this provides sufficient accuracy for the limited and homogeneously distributed deadtime in these measurements, we recalculate $\nu_{\text{max}}$ according to the updated model (see Table 3).

2.7. HM ensemble evaluation

The HMs of the IST system are distributed across multiple rooms and operate in a well-controlled environment. We expect their stochastic behaviour to be independent. Long-term observation by DMTD comparisons confirm similar behaviour and instabilities. Using the hourly data set spanning multiple years, we calculate Hadamard variances for the frequency difference $\dot{\gamma}_{A,B} = \gamma_A - \gamma_B$ of each pair of HMs A and B. The longest common operating interval is used for this, and only frequency excursions $> 5 \times 10^{-14}$ are rejected as outliers. Such outliers typically result from maintenance work or similar external disturbances and make up no more than 0.5% of the data for the HMs investigated. We average the variances weighted by the length of valid data and divide by 2 to determine an ensemble-average instability for a single HM. We fit this according to equation (6) with an additional WFN term and find $\sigma_H^2 (\tau) = \frac{4.2 \times 10^{-14}}{\sqrt{\tau/8}} + \left(2.1 \times 10^{-10}\right)^2 + \left((1.7 \times 10^{-17}) / \tau / 10^{-12}\right)^2$. The WFN contribution is in close agreement with the observations in measurements by NICT-Sr1.

We can leverage the ensemble of HMs to obtain a reduced uncertainty $\nu_{\text{max}} / \sqrt{N_{\text{ens}}}$ for $N_{\text{ens}}$ equally weighted HMs. This
is true even for the more complex noise processes such as flicker noise. Although these exhibit complex temporal correlations, they can be constructed from normally distributed contributions with arbitrary accuracy [31, 32].

To make use of the ensemble stability, we look at the frequency difference \( y_{HM,1}^{\Delta} \) of the reference HM (here HM_1) from the ensemble mean of the HM frequencies \( \bar{y}_{HM,j} \) recorded by the DMTD system relative to UTC(NICT) and averaged to 1 h intervals:

\[
y_{HM,1}^{\Delta} (t) = \bar{y}_{HM,1} (t) - \frac{1}{N_{ens}} \sum_{j=1}^{N_{ens}} y_{HM,j} (t). \tag{8}
\]

We obtain a linear fit \( y_{HM,1}^{\Delta} (t) \) over the evaluation period and subtract it from \( y_{HM,1}^{\Delta} (t) \) to eliminate both the mean value and the combined drift contributions. This defines a residual

\[
\delta y_{HM} (t) = y_{HM,1}^{\Delta} (t) - \bar{y}_{HM,1}^{\Delta} (t) \tag{9}
\]

as an estimate of the stochastic deviations of HM_1 from an ideal linear drift. This in turn is subtracted from the observations \( y_{yHM}^{\Delta} \) to generate ensemble-corrected time-series data

\[
y_{NR}^{\Delta} (t) = y_{obs}^{\Delta} (t) - \delta y_{HM} (t) \tag{10}
\]

that represents the behaviour of a noise-reduced virtual HM with the same mean frequency over the evaluation period. We then repeat the calculations of section 2.4 with \( y_{NR}^{\Delta} (t) \) replacing \( y_{obs}^{\Delta} (t) \). Figure 3 confirms the resulting reduction in instability, directly observed in the Hadamard deviation for \( \tau > 3600 \) s, the time step of \( y_{yHM}^{\Delta} \).

As constructed, \( \delta y_{HM} (t) \) integrates to zero over the full evaluation period, so that equation (10) only affects the results due to measurement deadtime. The resulting change in estimate \( y_{yHM} \) is generally within the range given by \( u_{stoc} \) and typically below \( 10^{-16} \) in magnitude. During the determination of \( \delta y_{HM} (t) \) we calculate frequency differences and Hadamard deviations to exclude HMs with degraded stability from the ensemble calculations. Table 3 lists \( N_{ens} \) for each evaluation.

2.8. Lab-side frequency determination

The uncertainty of the mean HM frequency \( \bar{y}_{yHM} \) over the chosen evaluation period is represented within the convention of the circular T, as also adopted in table 3, by the clock’s statistical uncertainty \( u_{\alpha} \), its systematic uncertainty \( u_{b} \) and the uncertainty \( u_{\beta}^{\alpha} \) in the link between the frequency standard and the reference clock implemented by the HM. This consists of the previously discussed contributions \( u_{\beta}^{\alpha} \) (section 2.4), \( u_{stat} \) (section 2.5), \( u_{stoc} \) (section 2.6) and \( u_{lab}^{\beta} \) (section 2.3) as:

\[
u_{\beta}^{\alpha} = u_{\beta}^{\alpha} + u_{stoc}^2 + u_{lab}^2 / N_{ens} + u_{lab}^2. \tag{11}
\]

Although the circular T has only recently begun reporting separate values for \( u_{\beta}^{\alpha} \) and \( u_{lab}^{\beta} \), the reports of NICT-Sr1 have always included a listing of \( u_{lab}^{\beta} \) as discussed in section 2.3. Over repeated measurements, the contributions grouped as \( u_{lab}^2 \) are expected to average according to the standard error of the mean. \( u_{lab}^{\beta} \) consists of a potential diurnal error that we treat as correlated across all measurements and a separate phase comparator error, correlated across all the earlier measurement it affects.

2.9. Frequency link to TAI

The phase of the reference HM is continuously compared to UTC(NICT), which is evaluated against UTC (and thus TAI, which is identical in frequency) through a GNSS link [33] with a timing instability of now typically \( \sigma_{link}^2 = 0.3 \) ns [20]. Time differences are calculated by BIPM for UTC 0:00 of modified Julian dates (MJD) ending in the digit 4 or 9. Relative frequencies can then be calculated over the intervening periods with a conventional uncertainty [21] of

\[
u_{Taul} = \sqrt{\frac{2\sigma_{link}^2}{T_0}} \left( \frac{T}{T_0} \right)^{0.9}, \tag{12}
\]

where \( T \) is the length of the evaluated period and \( T_0 = 5 \times 86400 \) s represents the 5 d interval. The exponent of 0.9 empirically accounts for long-term instabilities that exceed the fundamental \( 1/T \) behaviour expected for the white phase noise described by \( \sigma_{link}^2 \). Evaluated over typical 25 d to 35 d intervals, frequency standards commonly report \( u_{Taul} \approx 2 \times 10^{-16} \). The uncertainty of the HM–UTC(NICT) comparison is negligible.

2.10. Frequency trace to primary standards

For NICT-Sr1, the circular T data completes the frequency chain

\[
f(TAI) = f(SI) \cdot f(HM) \cdot f(Sr) / f(SI) \tag{13}
\]

The results are expressed in terms of the fractional deviation \( d \) of the scale interval \( 1/f(TAI) \) from the SI second

\[
d = \frac{f(SI)}{f(TAI)} - 1 \approx -\frac{f(TAI)}{f(SI)} = -\Delta y_{TAI}. \tag{14}
\]

Since \( d \) is typically of magnitude \( 1 \times 10^{-15} \), the approximation yields no loss in accuracy. Equivalent values are reported for all frequency standards contributing to TAI calibration, and we can trace from \( f(Sr) \) as measured by NICT-Sr1 to the results of a PFS by equating the results for \( d \) to obtain an expression for the Sr clock frequency in terms of the SI second:

\[
f(Sr) = f(SI) \cdot f(HM) / f(HM_S) \cdot f(TAI) / f(TAI_S) \cdot f(PFS) / f(SI) \tag{15}
\]

The HMs used as flywheel oscillators for the Sr and PFS measurements are differentiated by \( \alpha \) and \( \beta \). Each ratio term introduces uncertainty as discussed in the following. Most also represent measurements over specific intervals \( T \) that require extrapolation:
\[
\frac{f(Sr)}{f(SI)} = \frac{f(HM, T_{\alpha 1})}{f(HM, T_{\alpha 2})} \cdot \frac{f(TAI, T_{\alpha 2})}{f(TAI, T_{\alpha 1})} \cdot \frac{f(EAL, T_{\beta 2})}{f(EAL, T_{\beta 1})} \cdot \frac{f(HM, T_{\beta 1})}{f(HM, T_{\beta 2})} \cdot \frac{f(PFS)}{f(SI)}
\]  
\hspace{1cm} (16)

Here we extrapolate TAI by first converting to the underlying EAL which evolves continuously (see figure 4), while TAI is steered to match the SI second scale interval by stepwise corrections.

We can rewrite the equation as a sum of small fractional deviations \( y \) from the respective nominal values. For the Sr absolute frequency, the chosen nominal value is the 2017 CIPM recommendation for neutral \(^{87}\text{Sr}\) as SRS. \( f_{SRS}(\text{Sr}) = 429 \text{ 228 004 229 873 0 Hz} \) [7], such that

\[
f(\text{Sr}) = \left[ y \left( \frac{\text{Sr}}{\text{SI}} \right) + 1 \right] \cdot f_{SRS}(\text{Sr})
\]  
\hspace{1cm} (17)

Then

\[
y \left( \frac{\text{Sr}}{\text{SI}} \right) = -\left( y \frac{HM}{Sr, T_{\alpha 1}} + y \frac{HM}{Sr, T_{\alpha 2}} + y \frac{TAI}{HM, T_{\alpha 2}} \right) \text{ reported as } d \text{ in circular } T
\]

\[
-\left( y \frac{EAL}{TAI, T_{\alpha 2}} + y \frac{EAL}{EAL, T_{\beta 2}} + y \frac{EAL}{TAI, T_{\beta 2}} \right) \text{ reported in real – TAI and PFSs – TAI}
\]

\[
+\left( y \frac{HM}{PFS, T_{\beta 1}} + y \frac{HM}{HM, T_{\beta 2}} + y \frac{TAI}{HM, T_{\beta 1}} \right) \text{ reported as } d \text{ in circular } T
\]

\[
y \left( \frac{\text{Sr}}{\text{SI}} \right)
\]  
\hspace{1cm} (18)

All this data is publicly available from the BIPM FTP server [20]. The abbreviations ‘real–TAI’ and ‘PFSs–TAI’ refer to the reports ‘difference between the normalized frequencies of EAL and TAI’ and ‘difference between PSFS frequency and TAI frequency’.

For each evaluation of NICT-Sr1 as listed in table 3, we determine a value \( y(\text{Sr}/\text{SI}) \) for every PFS that reported a calibrating measurement with overlapping period. Seven of the evaluations were performed with frequent clock operation homogenously distributed over the full circular T reporting period. These achieve low uncertainties from the link to TAI as well as from extrapolation to the PFS evaluation through EAL. Here we use the reported value of \( d \) after applying a correction for the phase comparator error discussed in section 2.3. For five other evaluations, we make use of the improved HM characterization and extend the evaluation periods to more closely match the PFS data by recalculating \( d \) from the reported time difference UTC–UTC(NICT) and our records of HM–UTC(NICT). The same calculations were used to add an additional period representing four unreported clock operations between MJD 58 419 and 58 449.

The stochastic contribution to \( u_{b/\text{lab}} \) is now determined according to the model presented in section 2.6, and a minor adjustment has been applied to \( u_{b} \) for the re-evaluated servo error uncertainty (section 2.1). From March 2016 to March 2020, a total of 13 NICT-Sr1 evaluations in conjunction with reports of 8 Cs-fountain PFSs provide 63 datapoints \( y(\text{Sr}/\text{SI}) \) used to calculate the \(^{87}\text{Sr}\) absolute frequency.

2.11. Uncertainty contributions

For each of these datapoints, we identify 10 uncertainty contributions:

\( u_{\text{PFS}}^{S} \) and \( u_{\text{S}}^{S} \) are the statistical uncertainties of the measurements \( y(HM_{S}/PFS) \) and \( y(HM_{S}/\text{Sr}) \) resulting from the frequency standard itself. The corresponding errors are uncorrelated across separate measurements, but each measurement of NICT-Sr1 is compared to the results of multiple PFSs.

\( u_{\text{PFS}}^{\text{PS}} \) and \( u_{\text{S}}^{\text{PS}} \) describe the uncertainties for the satellite link of the local reference oscillator to TAI according to equation (12). Any constant equipment delays do not affect the frequency comparisons, and thus the uncertainties are taken to be uncorrelated for different periods. However, PFSs operated by the same institute share the same link, and there we assign a correlation coefficient of \( T_{\text{ov}}/\sqrt{T_{\alpha} - T_{\beta}} \) according to the length of the overlap \( T_{\text{ov}} \) in relation to the geometric mean of the individual intervals \( T_{\alpha} \) and \( T_{\beta} \) [34].

\( u_{b/\text{lab}} \) and \( u_{b/\text{lab}}^{S} \) characterize the additional uncertainty in transferring the measurements of the frequency standard to the flywheel oscillator measured against TAI, as discussed in section 2.8. For the PFS, we take the reported value \( u_{\text{PFS}}^{S} \) to predominantly represent the deadtime uncertainty of the extrapolation \( y(HM_{S}, T_{\beta 2}/HM_{S}, T_{\beta 1}) \) in equation (18) and to be statistically independent between measurements, as is \( u_{b/\text{lab}}^{S} \) for NICT-Sr1. We consider the contributions to \( u_{b/\text{lab}}^{S} \) to be fully correlated across all measurements.

The final contribution \( u_{c/\text{lab}} \) describes the uncertainty of extrapolating from interval \( T_{\alpha 2} \) to \( T_{\beta 2} \) using EAL as flywheel with an instability of

\[
\sigma_{c}^{2}(\tau) = 3 \times 10^{-30} (\tau/d)^{-1} + 12 \times 10^{-32} + 4 \times 10^{-34} (\tau/d)
\]  
\hspace{1cm} (19)

up to MJD 57 809, and

\[
\sigma_{c}^{2}(\tau) = 2 \times 10^{-30} (\tau/d)^{-1} + 9 \times 10^{-32} + 4 \times 10^{-34} (\tau/d)
\]  
\hspace{1cm} (20)

after that. These values are given monthly in the report ‘fractional frequency of EAL from PFS’ [20] and we calculate a PSD \( S_{b}^{EAL} \) for the combination of WFN, FFN and RWFM.
Figure 4. Overview of results. (a) For 13 TAI evaluation periods of NICT-Sr1, all 63 overlapping PFS reports (coloured symbols) were evaluated to find the absolute frequency. The reported deviations of the TAI scale interval $d$ were converted to a deviation $y$ (EAL) to remove the stepwise corrections applied to TAI (line). Error bars indicate total 1$\sigma$ uncertainties of the evaluation. The results of NICT-Sr1 are shown by offset brackets for visibility over the PFS datapoints. The darkly shaded region indicates the 1$\sigma$ uncertainty band for the BIPM estimate of $y$ (EAL), interpolated to illustrate the continuous behaviour. Horizontal bars at the bottom indicate the evaluation periods of the frequency standards relevant to this evaluation, spanning March 2016 to March 2020. (b) Averaged results for individual NICT-Sr1 evaluations in terms of the fractional deviation $y_{(Sr/SI)}$ from the nominal value $f_{SRS}$ (Sr). Error bars indicate overall uncertainty, with additional smaller marks indicating the reduced variance $v_{rv}$ expected relative to the weighted mean, as described in section 3. Percentages give the contributions to the overall mean displayed as the black line, with the orange-shaded region indicating a 1$\sigma$ uncertainty of $1.8 \times 10^{-16}$. (c) Results grouped by referenced PFS and averaged over evaluation periods. Percentages represent relative contributions. Error bars indicate overall uncertainty of the average, with smaller marks indicating $v_{rv}$ relative to the mean. Although the results for SU-CsF02 show a larger than expected deviation, the reduced $\chi^2$ is 0.51.

2.12. Covariance and weights

Given the vector $y$ constructed from the 63 individual values $y_{(Sr/SI)}$, the mean value weighted according to the column vector of normalized weights $w$ is simply $\bar{y}_{(Sr/SI)} = w^T y$. The corresponding uncertainty is described by a variance

$$\sigma^2 = w^T C w,$$

where the $63 \times 63$ covariance matrix $C$ describes the error correlations. Here and in the following, superscripts of T and $-1$ mark transposals and inversion.
We construct $C$ as the sum of individual matrices $C_i$ for each of the ten uncertainty contributions discussed in the previous section. Each $C_i$ is simply constructed by combining the reported uncertainties with a correlation matrix containing coefficients of 0 for uncorrelated contributions and 1 for correlated contributions. For example, the correlation matrix for the NICT-Sr1 systematic uncertainty contribution consists entirely of ones, which results in an uncertainty that does not decrease with the addition of more data. Fractional correlation coefficients are assigned where there is a partial overlap of measurement data [34].

For a known covariance matrix $C$, the optimization problem to find optimal weights $w_{op}$ is solved by the Gauss–Markov theorem:

$$w_{op} = \sigma_{op}^2 j^T C^{-1}, \quad \sigma_{op}^2 = (j^T C^{-1} j)^{-1}.$$  \hfill (22)

The design matrix $j$ is the column vector of ones $j = (1, 1, \ldots, 1)^T$. $w_{op}$ is optimal under the condition that knowledge of $C$ is complete. We find a slight complication in that, for the conservative assumption of strongly correlated errors, equation (22) yields very uneven weights among repeated measurements referencing the same PFSs. Uncorrelated uncertainty contributions typically favour distributed weights, but among those listed in section 2.11, only $u_{u}^{PFS}$ and $u_{w}^{PFS}$ are statistically independent over all 63 values for $\gamma$(Sr/SI). We consider this concentration of weights undesirable as it increases the sensitivity of the mean value to undiagnosed frequency excursions during the over-weighted measurements, and because the type b uncertainties of the frequency standards are still expected to have time-varying components that would tend to average out, even if this is not reflected in the uncertainty budget. For this reason, we apply a formally sub-optimal, but more evenly distribution of weights. We temporarily assign a reduced correlation coefficient of 0.5 for the systematic uncertainty of the same PFS in separate measurements to calculate a hypothetical covariance matrix $C$. This is used only to determine a set of weights $w'$ according to equation (22) and find $\gamma$(Sr/SI) = $w'^T y$ along with the accompanying uncertainty $\sigma'^2 = w'^T C w'$, where the original, conservative covariance matrix $C$ is used. Although $w'$ is not formally optimal for this matrix, the increase in uncertainty is minimal, as shown below. The distribution of weights across PFSs and evaluation periods is included in figure 4.

### Table 4. Uncertainty budget of frequency evaluation.

| Contribution                        | Symbol | NICT-Sr1 ($\times 10^{-16}$) | PFS ($\times 10^{-16}$) |
|-------------------------------------|--------|------------------------------|-------------------------|
| Clock statistical unc.              | $u_a$  | 0.06                         | 0.27                    |
| Clock systematic unc.               | $u_b$  | 0.72                         | 1.03                    |
| Link to local reference             | $u_{lab}$ | 0.68                         | 0.12                    |
| systematic contribution             | $u_{sys}$ | 0.58                         | n.a.                    |
| Satellite link to TAI               | $u_{TAI}$ | 0.65                         | 0.34                    |
| Clock evaluation totals             | $u_{ext}$ | 1.32                         | 1.13                    |
| EAL extrapolation                   |        |                              |                         |
| Overall uncertainty                 | $u_{ext}$ | 1.77                         |                         |

### 3. Results

Applying $w'$ to the matrices $C_i$ representing individual uncertainty contributions yields the uncertainty budget in table 4. The systematic uncertainties of the eight contributing PFSs give a combined $u_{sys}^{PFS} = 1.03 \times 10^{-16}$, similar to the values obtained in recent evaluations that trace the frequency of optical standards to TAI [10, 11, 16].

The overall fractional uncertainty of the mean is $u_{ext} = 1.77 \times 10^{-16}$ for the more evenly distributed weights $w'$. Applying the formally optimal weights $w_{op}$ would only result in a reduction to $1.74 \times 10^{-16}$.

Over the full set of datapoints, we find a reduced $\chi^2 = 0.45$, although this does not account for the expected correlations of the results. As an alternative measure of overall statistical consistency, we consider a reduced variance in the form of vector $v_{rv} = \text{diag}(C) - C w'$. This describes individual variances $v_{rv,j}$ corrected for covariance with the correctly weighted mean. Applying $w'$ to the standardized residuals $\Delta v_{rv,j}$ then gives

$$X_{rv}^2 = \sum_i w_i \frac{\Delta v_{rv,j}}{v_{rv,j}} = 0.43,$$  \hfill (23)

which is likewise consistent with a purely statistical variation. As shown in figure 4, we can also separate the results into contributions from individual evaluation of NICT-Sr1 and for individual PFSs. Averaged over evaluations, we find $\chi^2 = 0.39$ ($X_{rv}^2 = 0.38$), while over PFSs $\chi^2 = 0.51$ ($X_{rv} = 0.57$). Although we observe the contribution of SU-CsFO2 to deviate by 1.7$\sigma$ from the mean, such a deviation is expected with 55% probability over the eight PFS contributions. Overall, the uncertainties listed in the circular T appear to be rather conservatively estimated.

We then find a weighted mean $\bar{\gamma}$ (Sr/SI) = 1.92 (1.77) $\times 10^{-16}$. This fractional deviation from the nominal value $f_{SR}$(Sr) = 429 228 004 229 873.0 Hz in equation (17) represents an absolute $87^{\text{Sr}}$ frequency of $f$(Sr) = 429 228 004 229 873 082 (76) Hz obtained by comparisons of NICT-Sr1 to the PFSs contributing to TAI calibration.

### 4. Discussion

This new evaluation is consistent with our earlier absolute frequency measurements [15, 17, 18] and improves on the most
recent result with a reduction in overall uncertainty by a factor of 2.4. Since there have been only limited changes to the evaluation of systematic frequency shifts in NICT-Sr1, and parts of the evaluated period overlap, the new result should be considered a replacement of earlier data rather than an independent contribution.

Two other institutes have recently reported updates to their determination of the Sr frequency (table 5), by comparison to TAI [35], and against local PFSs [16]. Some of the most stringent tests of optical clocks now take the form of loop closures [10, 36]. The Yb/Sr frequency ratio has recently been re-determined [37] as $R = 1.2075070393433378482(82)$, with $7 \times 10^{-18}$ fractional uncertainty. Even though this differs by 1.8σ from previous results [38], the fractional difference is only $8 \times 10^{-17}$, significantly below the uncertainties of the absolute frequency measurements. This allows us to additionally consider two new results for the absolute frequency of the $^{171}$Yb clock transition [10, 11]. The comparison values are included in table 5 together with corresponding $ar{f}_{Sr} = f_{Yb}/R$, where $R$ now contributes negligible uncertainty. Both Yb results also reference the ensemble of PFSs contributing to TAI calibration, and for the period of their determination state corresponding uncertainties of $1.3 \times 10^{-16}$ and $1.2 \times 10^{-16}$. Taking the remaining contributions to be statistically independent, we find a mean value $f_{Yb} = 518\,295\,836\,590\,863.67(10)$ Hz. With $R$ and our value for $f_{Sr}$, this yields a misclosure

$$
\delta = \frac{f_{Yb}/f_{Sr}}{R} = -1.4(2.6) \times 10^{-16},
$$

well within statistical expectations. It is reasonable to expect that systematic frequency errors in the near-identical ensemble of referenced PFSs are largely identical for all three evaluations. A complete cancelation would reduce the uncertainty to $2.0 \times 10^{-16}$, which remains consistent with the observed misclosure.

5. Conclusion

Figure 5 illustrates the excellent agreement of the various results, as well as the progression of uncertainties of the CIPM recommended frequencies for neutral strontium and ytterbium as secondary representations of the second. Results as presented here, finding agreement between international measurements both in absolute frequency and through the growing matrix of optical-to-optical comparisons, now support a further uncertainty reduction. If the CIPM were to adopt a new recommendation for the $^{87}$Sr clock transition frequency that reduces the uncertainty $u_{g_{0S}}$ from its present value of $4 \times 10^{-16}$ to $1.8 \times 10^{-16}$, as we find in our evaluation, it

| Source       | Reference | $^{87}$Sr absolute frequency (Hz) | Additional information       |
|--------------|-----------|----------------------------------|------------------------------|
| NICT         | (JP)      | 429 228 004 229 873.08(08)        | $1.8 \times 10^{-16}$ fractional uncertainty |
| PTB          | (DE)      | 429 228 004 229 873.00(07)        | $1.5 \times 10^{-16}$ fractional uncertainty |
| NPL          | (UK)      | 429 228 004 229 873.1(5)          | $1.2 \times 10^{-15}$ fractional uncertainty |
| CIPM 2017    |           | 429 228 004 229 873.00(17)        | Secondary representation of the second |
| JILA         | (US)      | 429 228 004 229 873.04(09)        | $R = 1.207\,507\,039\,343\,337\,848\,2(82)$ |
| Yb: NIST     | (US)      | (See above)                       | $f_{Yb} = 518\,295\,836\,590\,863.71(11)$ Hz |
| Yb: INRIM    | (IT)      | 429 228 004 229 872.99(11)        | $f_{Yb} = 518\,295\,836\,590\,863.61(13)$ Hz |

Figure 5. Comparison of results. The main figure shows the progression of the CIPM recommended frequencies for $^{87}$Sr (horizontal) and $^{171}$Yb (vertical) as coloured ellipses. All values are plotted relative to the 2017 CIPM recommendation. Measurements of the absolute frequencies [10, 11, 16, 35] reported later than this are shown by open circles and error bars to the left and below. The result reported here (solid point below) is in good agreement with the 2017 CIPM recommendation (shaded areas indicate the 1σ confidence interval) and the recent measurements. The diagonal blue line in the main figure represents the confidence interval of a precise optical-to-optical measurement of the Yb/Sr frequency ratio [37]. The white overlaid ellipse shows the combined uncertainties of the mean of the Yb results (see text) and our measurement of the Sr frequency, as used in the closure calculation.
would permit optical clocks like NICT-Sr1 (with average $\nu_b = 7.3 \times 10^{-17}$) to contribute to the steering of TAI with an effective systematic uncertainty $\nu_{b\text{eff}} = \sqrt{\nu_b^2 + \nu_{bSR}^2} < 2 \times 10^{-16}$. This outperforms all PFSs considered in this evaluation apart from PTB-CSF2 and IT-CSF2 (both of which report $\nu_b = 1.7 \times 10^{-15}$), establishing optical clocks as first tier members of the TAI steering ensemble.

Directly tracing a frequency chain to individual frequency standards helps minimize the uncertainty from mismatched evaluation periods. It also allows us to reference specific, pri-

tives systematic uncertainty

assigned to each standard, as included in figure 4. This will facilitate calculations that need to account for correlations between results [34]. As optical clocks gain increased weight in the steering of TAI, such additional care is required to make sure absolute frequency determinations are correctly traced to the SI second and the PFSs that implement it according to definition.

Our results were obtained using the same measurements, frequency links and communication channels used in the steering of the international time scale. Where local clock comparisons rely only on the local infrastructure, our results demonstrate accuracy and stability for the complete measurement chain.

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