BIPM Workshop on Measurement Uncertainty
16 June 2015

The 2014 CODATA determination of the best values and uncertainties of the fundamental constants

David B. Newell
National Institute of Standards and Technology
Gaithersburg, MD, USA

Outline

- Past adjustments of the constants
- Role and methodology of CODATA TGFC
- 2014 Least Squares Adjustment
- CODATA and the new SI

Past – before CODATA

- ## Method of Least Squares
  - “Nouvelles méthodes pour la détermination des orites des comètes,” Adrien-Marie Legendre, Paris, publisher F. Didot, (1805)
  - “Theoria motus corporum coelestium in sectionibus conicis solem ambientium,” C. F. Gauss, Hamburg: S. F. Perthes and I. H. Besser, (1809)
  - “Théorie Analytique des Probabilités,” P. S. Laplace, marquis de, vol. II, Paris: Ve. Courcier, (1812)
  - “Theoria Combinationis Observationum Erroribus Minimis Obnoxiae,” in Commentationes societatis regiae scientiarum Gottingensis recentiores, Vol. v., C. F. Gauss, Göttingen: Royal Society of Göttingen, pp. 33-62 (1823)

- ## Adjustments of the Constants
  - “Probable Values of the General Physical Constants,” R. T. Birge, Rev. Mod. Phys. **1**(1), 1-73 (1929)

Past– before CODATA

• Subsequent determinations

- "Our Knowledge of the Atomic Constants F, N, m, and h in 1947, and of Other Constants Derivable Therefrom," J. W. M. DuMond and E. R. Cohen, Rev. Mod. Phys. **20**(1), 82-108 (1948) E **21**(4), 651-652 p. (1949)
- "A Re-Evaluation of the Fundamental Atomic Constants," J. A. Bearden and H. M. Watts, Phys. Rev. **81**(1), 73-81 (1951)
- "Least-Squares Adjustment of the Atomic Constants, 1952," J. W. M. DuMond and E. R. Cohen, Rev. Mod. Phys. **25**(3), 691-708 (1953)
- "Present Status of the Atomic Constants," J. A. Bearden, M. D. Earle, J. M. Minkowski, and J. S. Thomsen, Phys. Rev. **93**(3), 629-630 (1954)
- "A Survey of Atomic Constants," J. A. Bearden and J. S. Thomsen, Nuovo Cimento Suppl. **5**(2), 267-360 (1957)
- "A survey of the systematic evaluation of the universal physical constants," R. T. Birge, Nuovo Cimento Suppl. **6**(1), 39-67 (1957)
- "Résumé of Atomic Constants," J. A. Bearden and J. S. Thomsen, Am. J. Phys. **27**(8), 569-576 (1959)
- "Status of Knowledge of the Fundamental Constants of Physics and Chemistry as of January 1959," J. W. M. DuMond, Ann. Phys. (N.Y.) **7**(4), 365-403 (1959)
- "Our Knowledge of the Fundamental Constants of Physics and Chemistry in 1965," E. R. Cohen and J. W. M. DuMond, Rev. Mod. Phys. **37**(4), 537-594 (1965)
- "Determination of e/h, Using Macroscopic Quantum Phase Coherence in Superconductors: Implications for Quantum Electrodynamics and the Fundamental Physical Constants," B. N. Taylor, W. H. Parker, and D. N. Langenberg, Rev. Mod. Phys. **41**(3), 375-496 (1969)

Treatment of Discrepant Data

- **Expand all uncertainties for a satisfactory χ^2**
- **Exclude "incompatible" data, no expansion**
-
-

"Comments on Least-Squares Adjustments of The Constants," B. N. Taylor, Proceedings of the International Conference on Precision Measurement and Fundamental Constants, NBS, Gaithersburg, MD, August 3-7, 1970

Treatment of Discrepant Data

- **Expand all uncertainties for a satisfactory χ^2**
- **Exclude "incompatible" data, no expansion**

:

A set of constants is needed, 'tis true,
And we must give the adjusters their due.
But why can't they see
How better it would be
If they'd used my experiment too!

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- .

A set of constants is needed, 'tis true,
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But why can't they see
How better it would be
If they'd used my ~~experiment~~ analysis too!

- **Input data must be thoroughly investigated!**

"Comments on Least-Squares Adjustments of The Constants," B. N. Taylor, Proceedings of the International Conference on Precision Measurement and Fundamental Constants, NBS, Gaithersburg, MD, August 3-7, 1970

Formation of CODATA

- **1966 –ICSU establishes the Committee on Data for Science and Technology (CODATA)**
  - To strengthen international science for the benefit of society by promoting improved scientific and technical data management and use

ICSU
International Council for Science
icsu.org

- **1969 CODATA establishes the Task Group on Fundamental Constants**
  - To periodically provide the scientific and technological communities with a self-consistent set of internationally recommended values of the basic constants and conversion factors of physics and chemistry based on all of the relevant data available at a given point in time.

codata.org

CODATA Adjustments

- "The 1973 least-squares adjustment of the fundamental constants," E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2(4), 663-734 (1973)
- "The 1986 adjustment of the fundamental physical constants," E. R. Cohen and B. N. Taylor, Rev. Mod. Phys. 59(4), 1121-1148 (1987)
- "CODATA recommended values of the fundamental physical constants: 1998," P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **72**(2), 351-495 (2000)
- "CODATA recommended values of the fundamental physical constants: 2002," P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **77**(1), 1-107 (2005)
- "CODATA recommended values of the fundamental physical constants: 2006," P. J. Mohr, B. N. Taylor, and D. B. Newell, Rev. Mod. Phys. **80**(2), 633-730 (2008)
- "CODATA recommended values of the fundamental physical constants: 2010," P. J. Mohr, B. N. Taylor, and D. B. Newell, Rev. Mod. Phys. **84**(4), 1527-1605 (2012)

The NIST Reference on Constants, Units, and Uncertainty

Information at the foundation of modern science and technology from the Physical Measurement Laboratory of NIST

CODATA Internationally recommended 2010 values of the Fundamental Physical Constants

pml.nist.gov/constants

Constants Topics:
- Values
- Energy Equivalents
- Searchable Bibliography
- Background

Constants Bibliography

Constants, Units & Uncertainty home page

Version history and disclaimer

(e.g., **electron mass**, most misspellings okay)

Search by name [ ] Search

Display ◉ alphabetical list, ○ table (image), or ○ table (pdf)

by clicking a category below

- Universal
- Electromagnetic
- Atomic and nuclear
- Physico-chemical
- Adopted values
- Non-SI units
- Conversion factors for energy equivalents
- X-ray values
- Frequently used constants
- Extensive listings
- All values (ascii)

Find the correlation coefficient between any pair of constants
Data from the least-squares adjustment of the values of the constants

See also

Article on the 2010 adjustment of the values of the constants
Searchable bibliography on the constants
Background information related to the constants
Links to selected scientific data
Previous Values (2006) (2002) (1998) (1986) (1973) (1969)
The CODATA 2014 values of the constants will be posted in Spring of 2015.

DEADLINE NOTICES!

There will be an adjustment of the constants to provide the values for a revision of the International System of Units (SI) expected to take place in 2018. To be considered for use in this adjustment, new results must be **accepted for publication by 1 July 2017**.

The 2018 CODATA adjustment of the fundamental constants will be based on the revised SI, which will significantly affect the uncertainties of many constants. For data to be considered for use in this adjustment, they must be **discussed in a publication preprint or a publication by 1 July 2018**.

Detailed contents About this reference Feedback Get the PDF Reader

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TGFC members

F. Cabiati, Istituto Nazionale di Ricerca Metrologica, Italy
J. Fischer, Physikalisch-Technische Bundesanstalt, Germany
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K. Fujii, National Metrology Institute of Japan, Japan
S. G. Karshenboim, D. I. Mendeleyev Institute of Metrology, Russia, and
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*Deceased

Outline

- Past adjustments of the constants
- **Role and methodology of CODATA TGFC**
- 2014 Least Squares Adjustment
- CODATA and the new SI

Role of CODATA TGFC

- **Provide the best values of the constants based on all relevant data available**
  - Smallest possible uncertainties
  - Unlike other data comparison analysis (i.e. - key comparisons) - no safety factors

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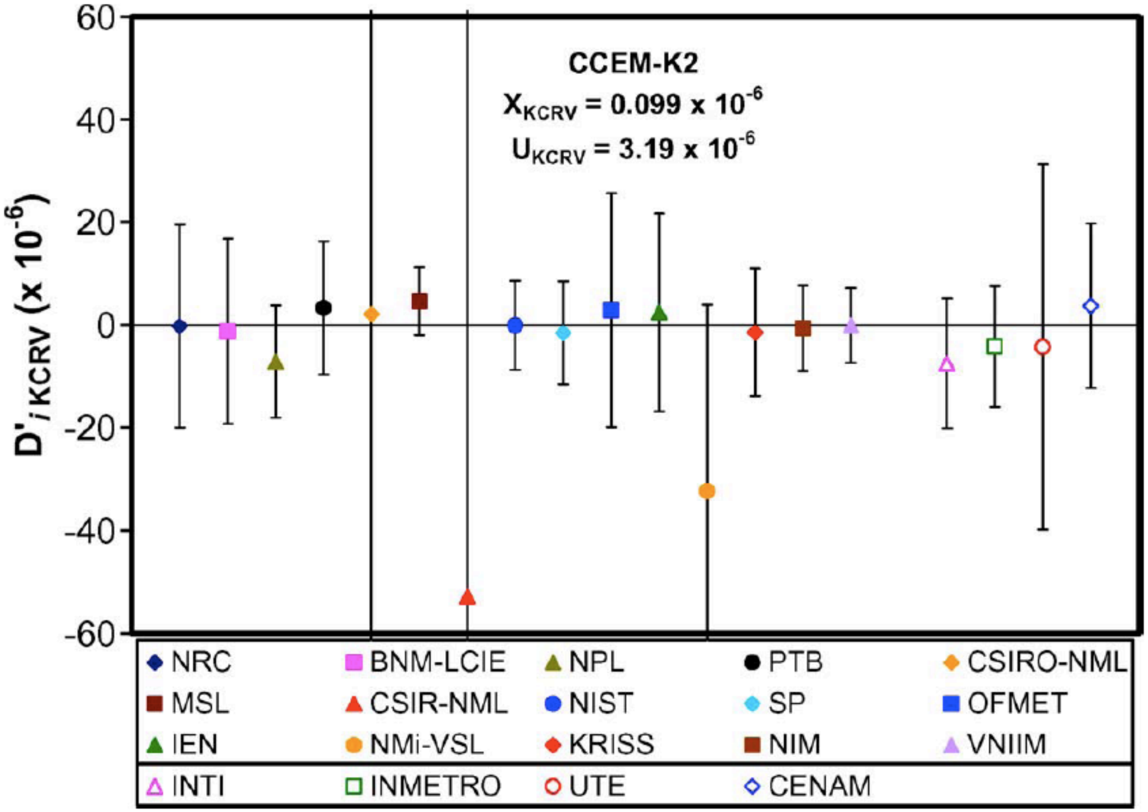
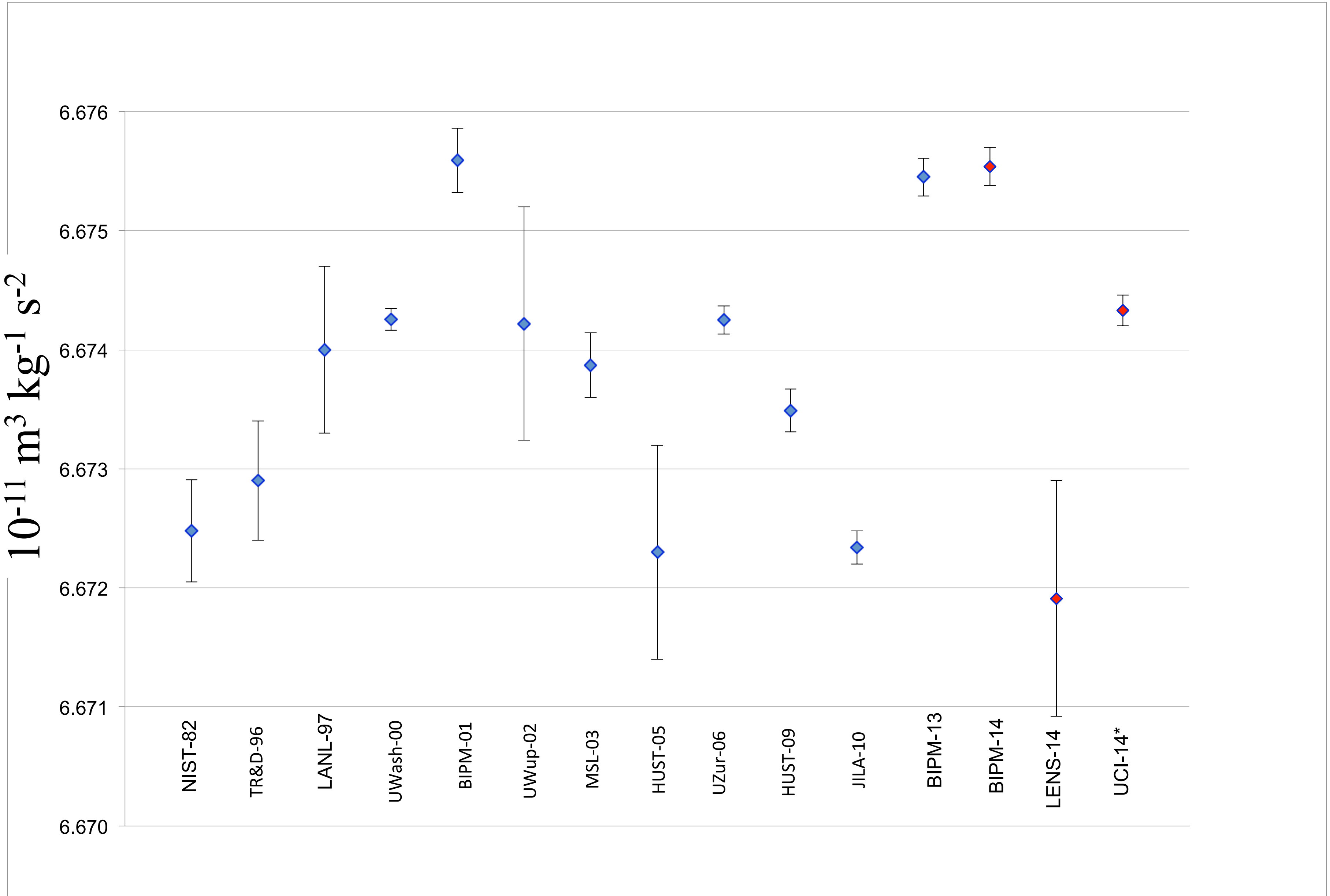


2014 Input data related to the Gravitational constant



A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

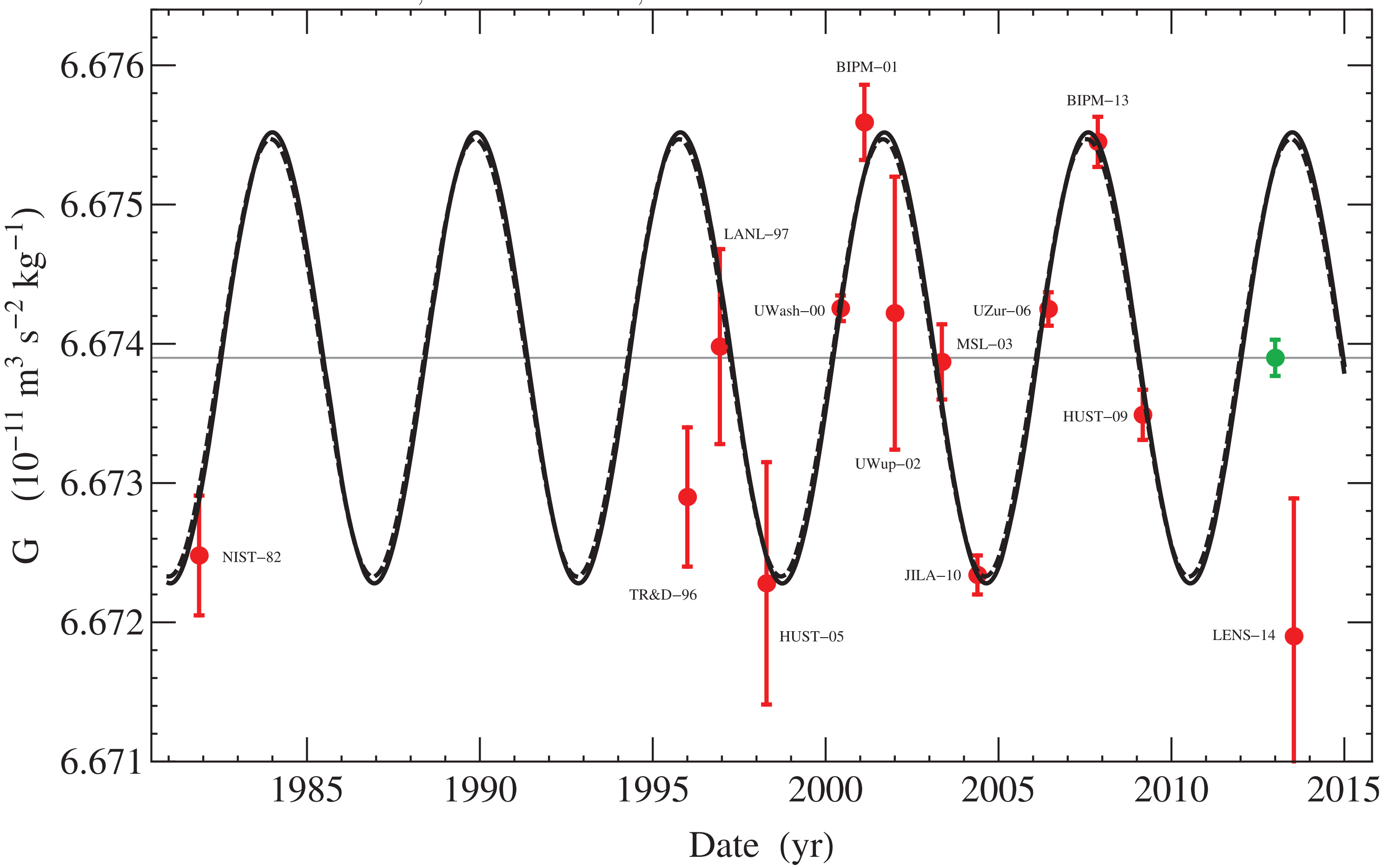
April 2015

EPL, **110** (2015) 10002
doi: 10.1209/0295-5075/110/10002

www.epljournal.org

Measurements of Newton's gravitational constant and the length of day

J. D. ANDERSON[1(a)], G. SCHUBERT[2], V. TRIMBLE[3] and M. R. FELDMAN[4]



Recent measurements of the gravitational constant as a function of time

S. Schlamminger

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Center for Experimental Physics and Astrophysics,
University of Washington, Seattle, WA 98195, USA

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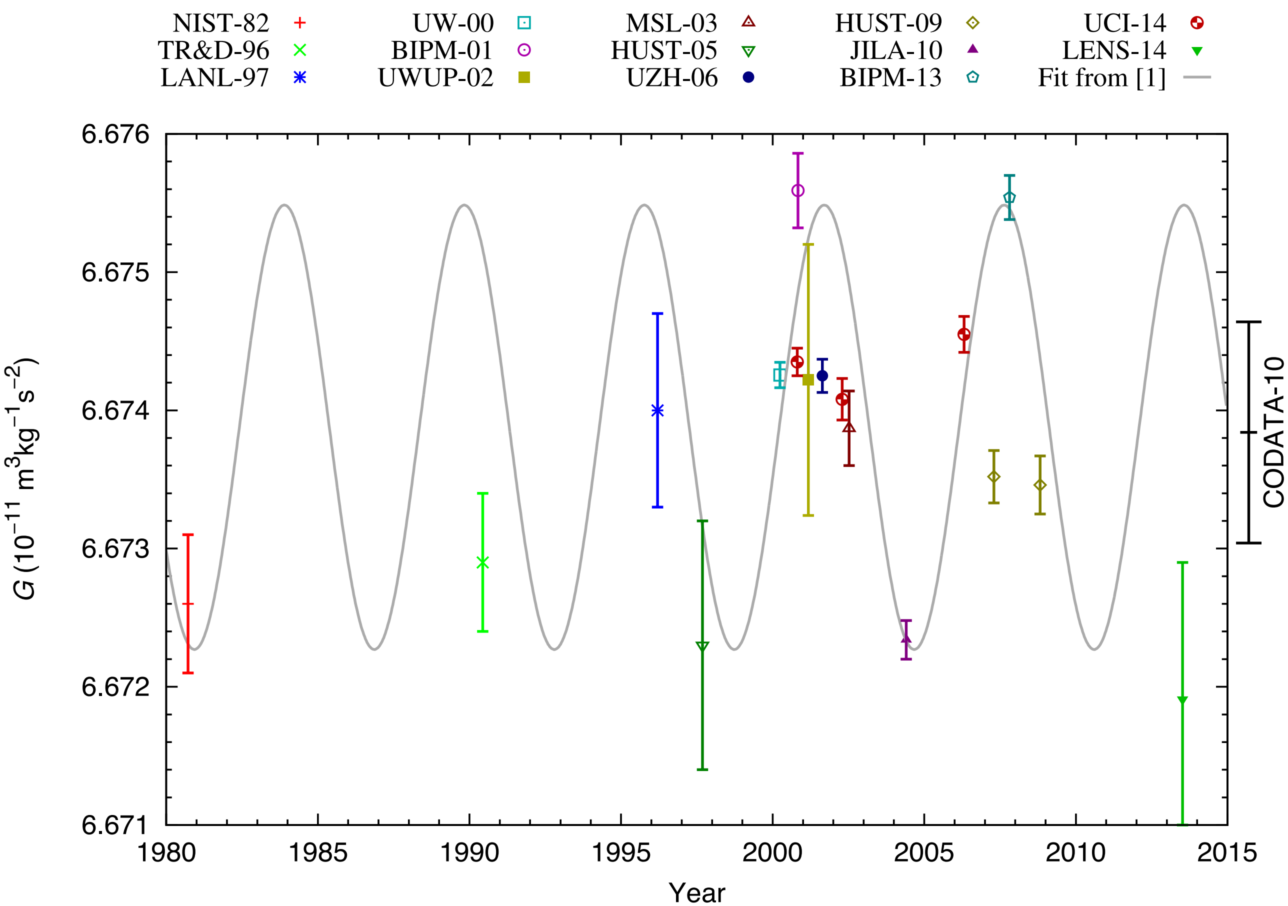
(Dated: June 10, 2015)



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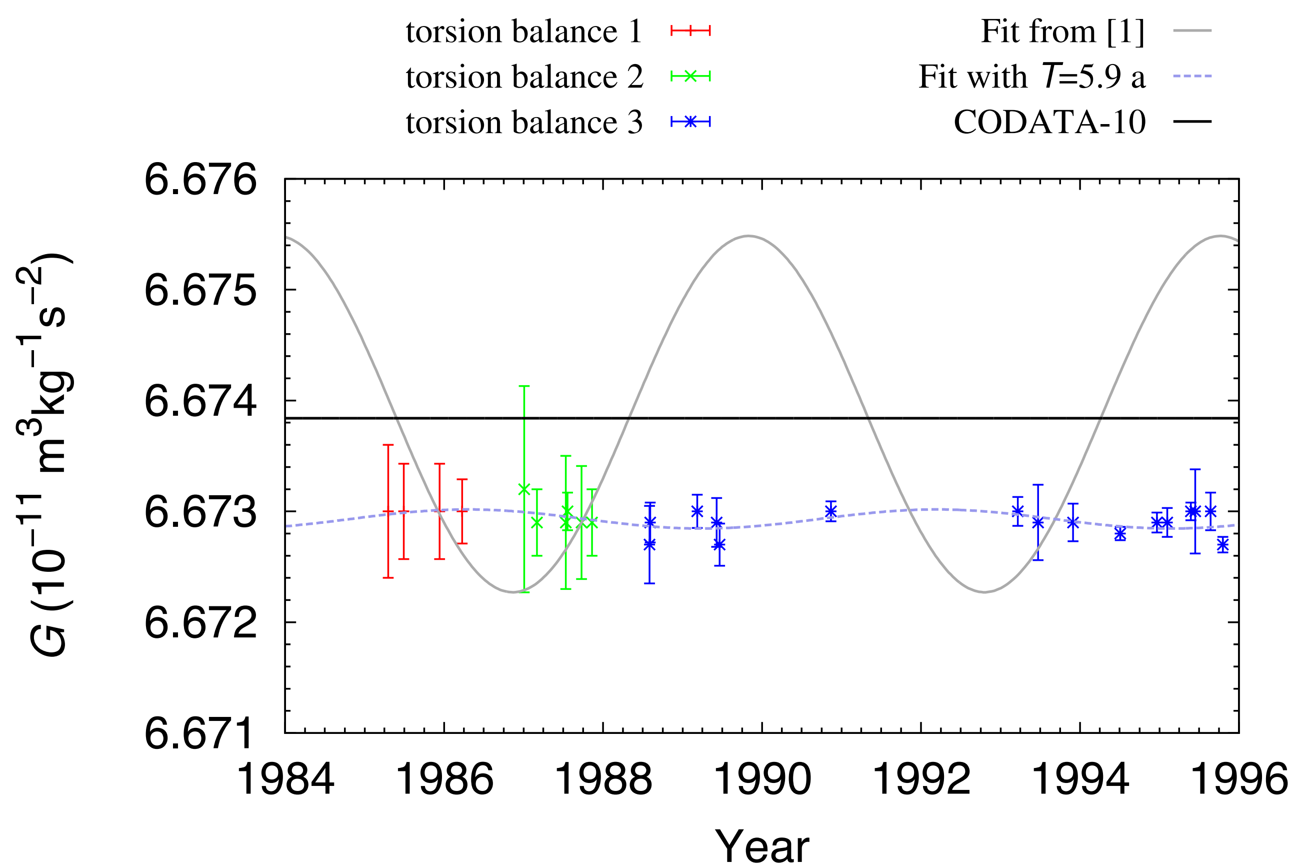

TGFC LSA Methodology

- **Collect all data**
  - Older data form previous LSAs
  - Include new data since the last LSA
- **Preliminary review of the data**
  - Check for up-to-date input and corrections
  - Full uncertainty analysis
  - Internal consistency
- **Assess relation with other input data**
  - Supersedes previous results?
  - Covariance - sort by common uncertainty components

TGFC LSA Methodology (cont.d)

- **Run mini LSA for each of the main constants and use "standard" statistic tools to investigate "goodness of fit"**
  - Chi squared (χ^2), Probability of reduced χ^2, Birge ratio R_B, Maximum Normalized Residuals (MNR), Maximum Normalized Difference (MND), etc.

$$\chi^2 = \sum \frac{(y_i - y_m)^2}{\sigma_{ii}^2} \qquad \sqrt{\chi^2/_{\upsilon}} \qquad \frac{(y_i - y_m)}{\sigma_{ii}} \qquad \frac{(y_i - y_m)}{(\sigma_{ii}^2 + \sigma_m^2)^{0.5}}$$

- **Adjust expansion factors, include/exclude specific data**
  - 1% self sensitivity test
- **Run "final" multi-variant LSA, argue, re-run LSA, etc.**
- ***Minimize total 'disagreement'***

Multivariable analysis

– Measured quantities (input data) expressed as theoretical functions of the constants (observational equations) through a particular independent subset of the constants (adjusted constants)

Examples of observational equations

$$K_J^2 R_K = \frac{4}{h}$$

$$N_A = \left(\frac{M_u c}{2}\right)\frac{A_r(e)\alpha^2}{R_\infty h}$$

$$R = R$$

$$k = \left(\frac{2}{M_u c}\right)\frac{R_\infty h R}{A_r(e)\alpha^2}$$

$$\frac{k}{h} = \left(\frac{2}{M_u c}\right)\frac{R_\infty R}{A_r(e)\alpha^2}$$

$$G = G$$

$$\nu_H\left(1S_{1/2} - 2S_{1/2}\right) = \frac{3}{4}R_\infty c\left[1 - \frac{m_e}{m_p} + \frac{11}{48}\alpha^2 - \frac{28}{9}\frac{\alpha^3}{\pi}\ln\alpha^{-2} - \frac{14}{9}\left(\frac{\alpha R_p}{ƛ_C}\right) + \dots\right]$$

Least Squares Formalism: Aitkins (1934)

observational data: $q_1,\ q_2, \ldots, q_N$

unknowns: $z_1,\ z_2, \ldots, z_M \qquad (M \le N)$

observational equations: $q_i \doteq f_i(z) \equiv f_i(z_1, z_2, \ldots, z_M)$

Linear approximation about starting values s for z:

$$q_i \doteq f_i(s) + \sum_{j=1}^{M} \frac{\partial f_i(s)}{\partial s_j}(z_j - s_j) + \cdots$$

or

$$y_i \doteq \sum_{j=1}^{M} A_{ij} x_j + \cdots$$

where $y_i = q_i - f_i(s)$, $x_j = z_j - s_j$,

and $A_{ij} = \dfrac{\partial f_i(s)}{\partial s_j}$

Least Squares Formalism: Aitkins (1934)

In matrix notation: $Y \doteq AX$

with *covariance matrix*: $V = \mathrm{cov}(Y)$

LSA is the solution $\hat{X}$ for X that minimizes

$$\chi^2(X) = (Y - AX)^\top V^{-1}(Y - AX)$$

If the observations Y are uncorrelated

$$(Y - AX)^\top V^{-1}(Y - AX) = \sum_{i=1}^{N} \frac{(Y - AX)_i^2}{(\delta Y)_i^2}$$

Solution:

$$\begin{aligned} \hat{X} &= (A^\top V^{-1} A)^{-1} A^\top V^{-1} Y \\ \mathrm{cov}(\hat{X}) &= (A^\top V^{-1} A)^{-1} \end{aligned}$$

and

$$\begin{aligned} \hat{Z} &= S + \hat{X} \\ \mathrm{cov}(\hat{Z}) &= \mathrm{cov}(\hat{X}) \\ \hat{Y} &= A\hat{X} \\ \hat{q}_i &= f_i(s) + \hat{y}_i \end{aligned}$$

Calculated constants

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

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

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

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- **2014 Least Squares Adjustment**
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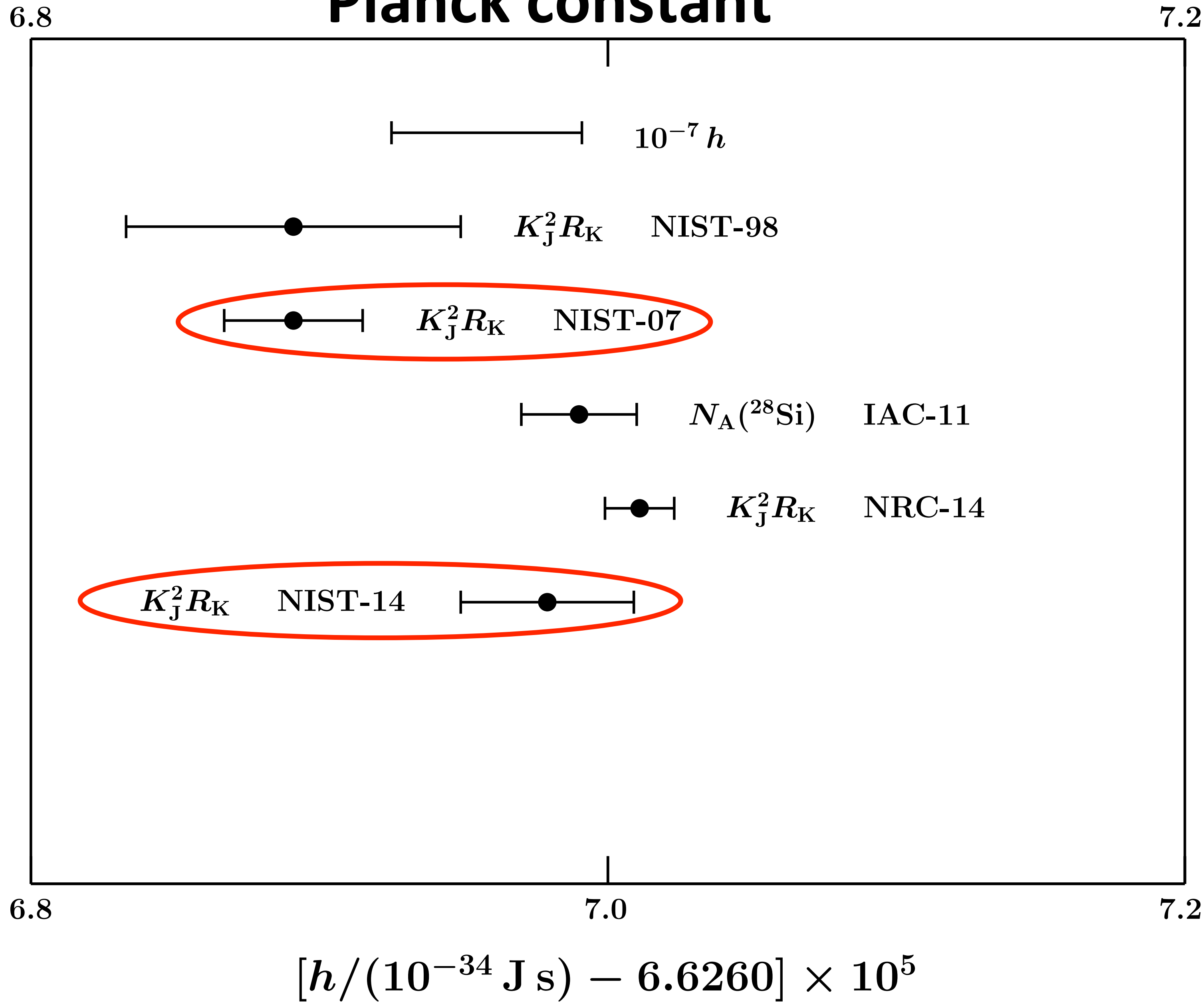
2014 Input data related to the Planck constant



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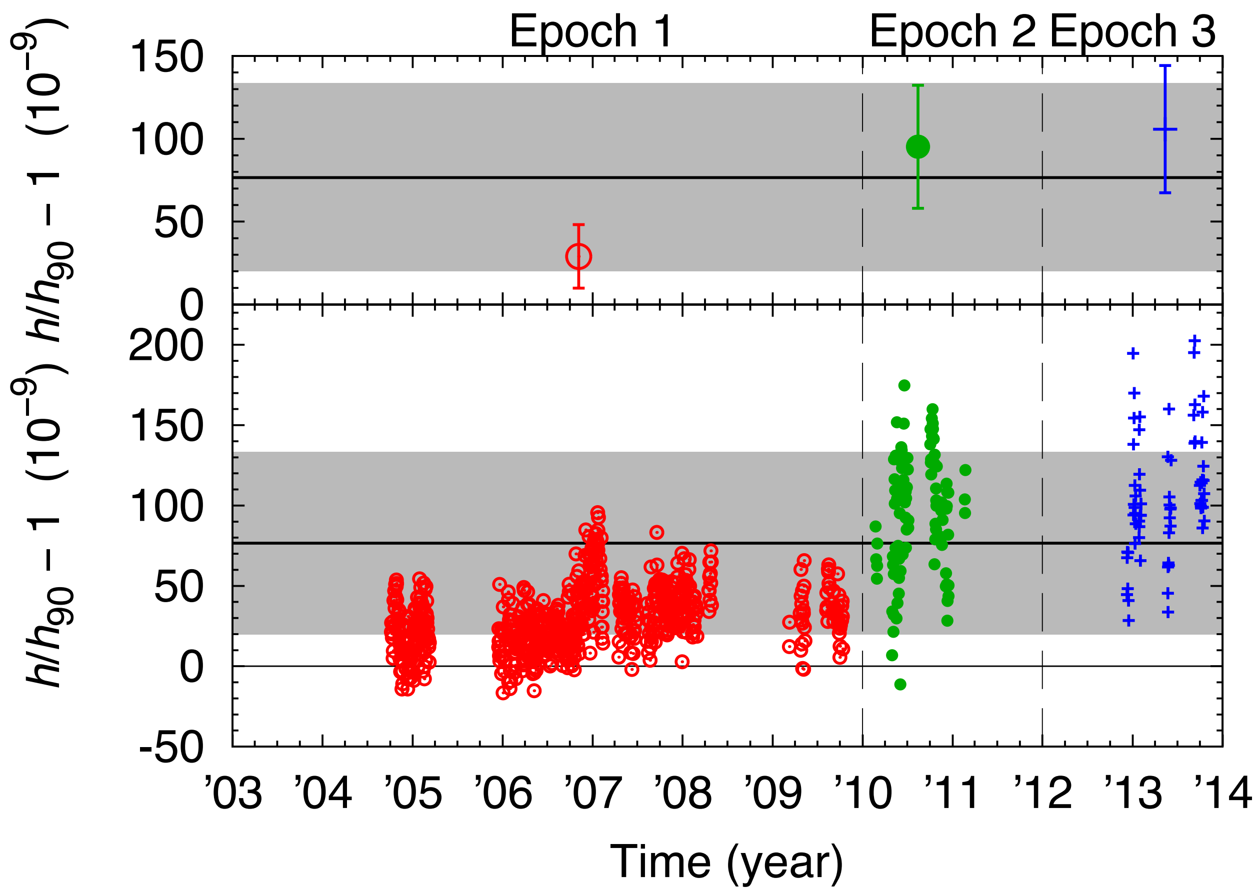
Metrologia
Metrologia **52** (2015) L5–L8
doi:10.1088/0026-1394/52/2/L5

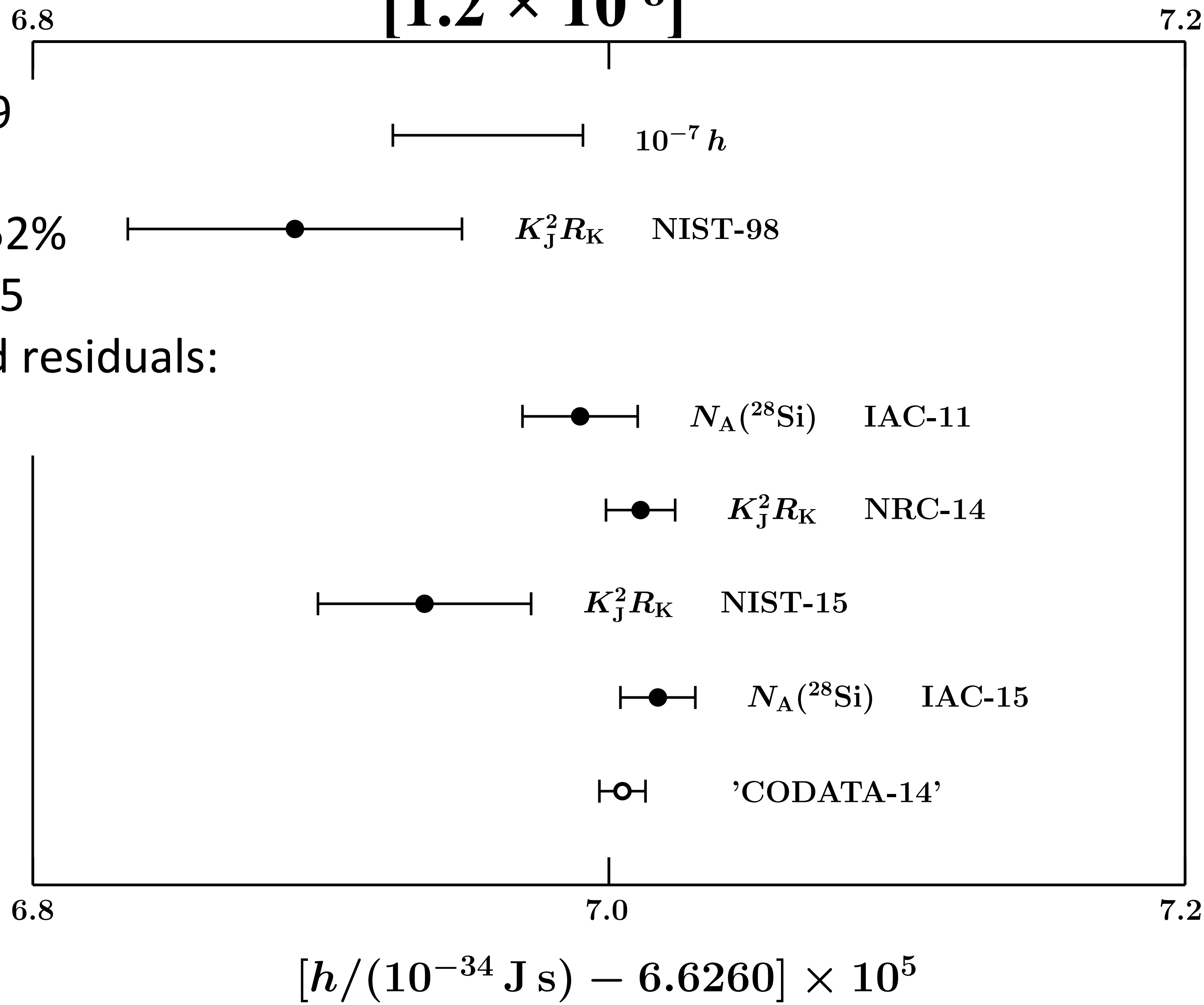
A summary of the Planck constant measurements using a watt balance with a superconducting solenoid at NIST

S Schlamminger[1], R L Steiner[1], D Haddad[2], D B Newell[1], F Seifert[2], L S Chao[1], R Liu[1], E R Williams[1] and J R Pratt[1]



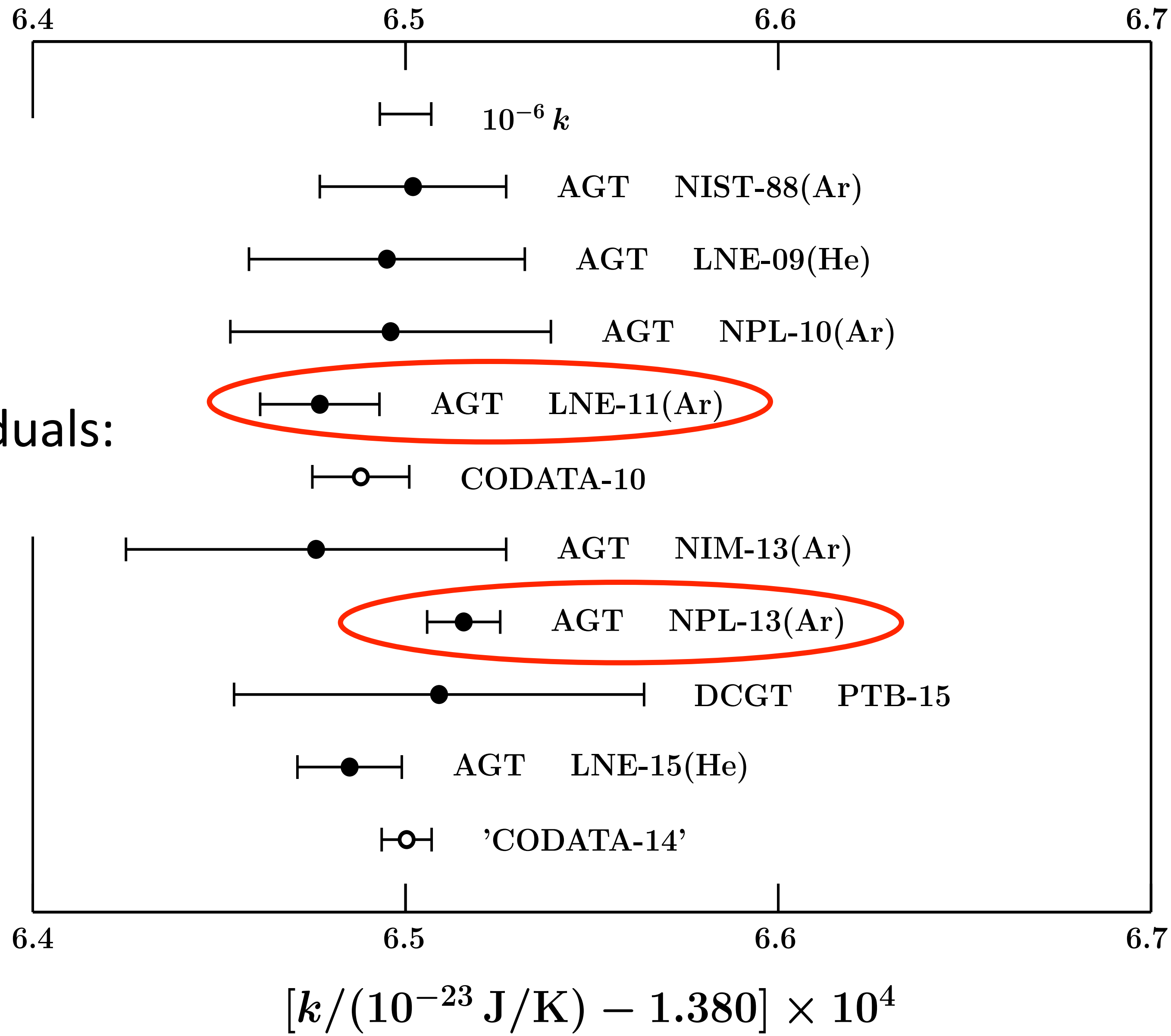
h = 6.626 070 038(81) × 10^{-34} J sec
[1.2 × 10^{-8}]

χ^2: 8.49
DOF: 4
Prob. χ^2: 7.52%
R_B: 1.45
Max. reduced residuals:
1.96, 1.84



2014 Input data related to the Boltzmann constant

χ^2: 5.50
DOF: 7
Prob. χ^2: 60.0%
R_B: 0.89
Max. reduced residuals:
-1.28, 1.55

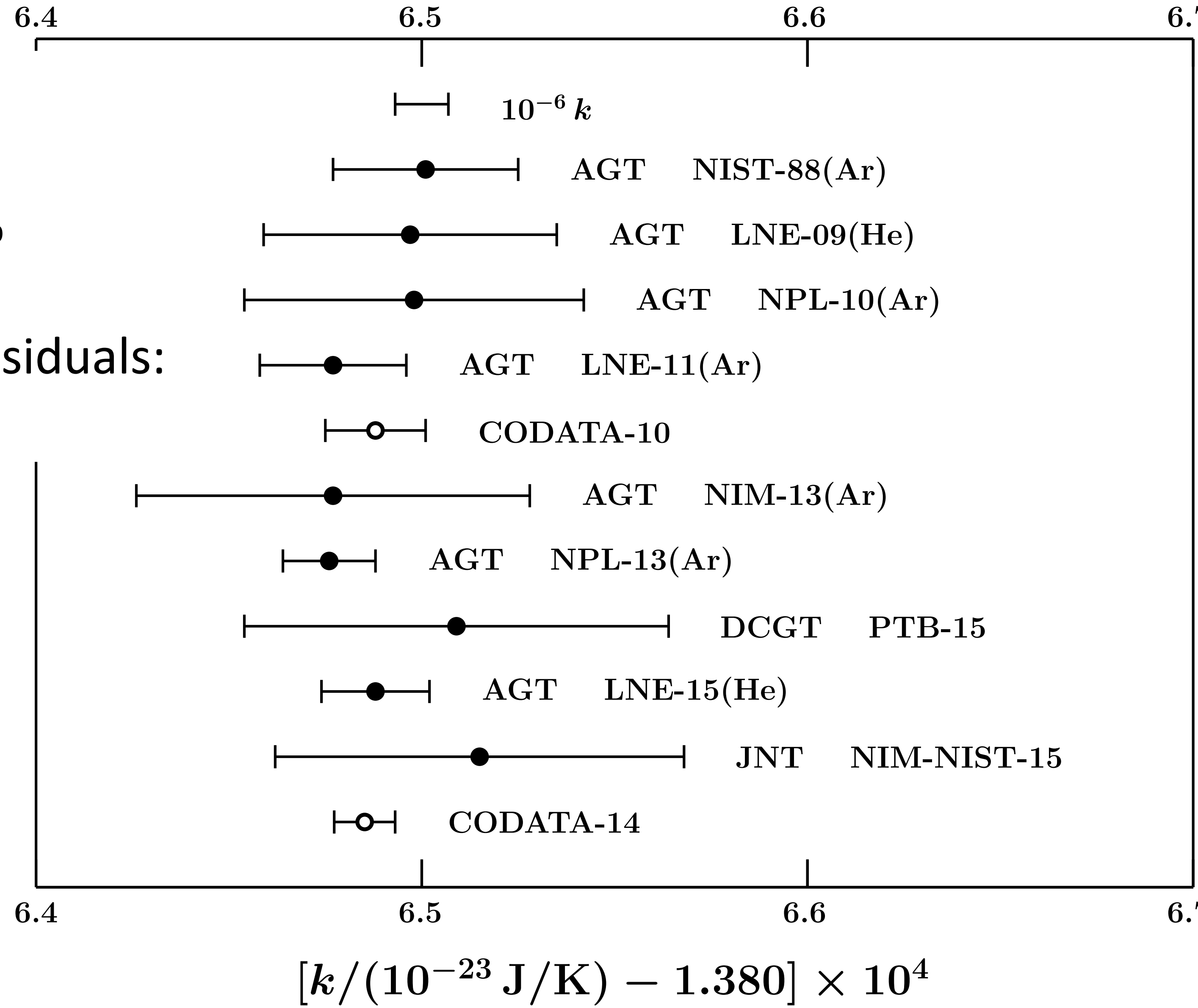


Acoustic Gas Thermometry Correlations

correlated relative uncertainty components, ppm	NIST-88 (Ar)	LNE-09 (He)	NPL-10 (Ar)	INRIM-10 (He)	LNE-11 (Ar)	NIM-13 (Ar)	NPL-13 (Ar)	LNE-15 (He)
mw geometry		0.05	0.05	0.01	0.05		0.05	0.05
mw waveguides and/or probe		0.10	0.10		0.10		0.10	0.10
fitting routine - NPL			0.02				0.02	
thermal cond Ar	0.02		0.02		0.02	0.02	0.02	
thermal cond He		0.02		0.02				0.02
acoustic geometry		0.05	0.05	0.01	0.05		0.05	0.05
A3 coefficient	0.05		0.05		0.07	0.07	0.08	
Molar mass He		0.10		0.17				0.10
Molar mass Ar - IRMM			0.70		0.70			
Molar mass Ar - KRISS						0.53	0.53	
Resonator Volume - LNE					0.57			0.57
TPW - LNE		0.16			0.16			0.16

$k = 1.380\ 648\ 52(79) \times 10^{-23}$ J K^{-1}
$[5.7 \times 10^{-7}]$

χ^2: 1.98
DOF: 8
Prob. χ^2: 98.0%
R_B: 0.50
Max. reduced residuals:
-0.72, 0.66



2014 Input data related to the Gravitational constant

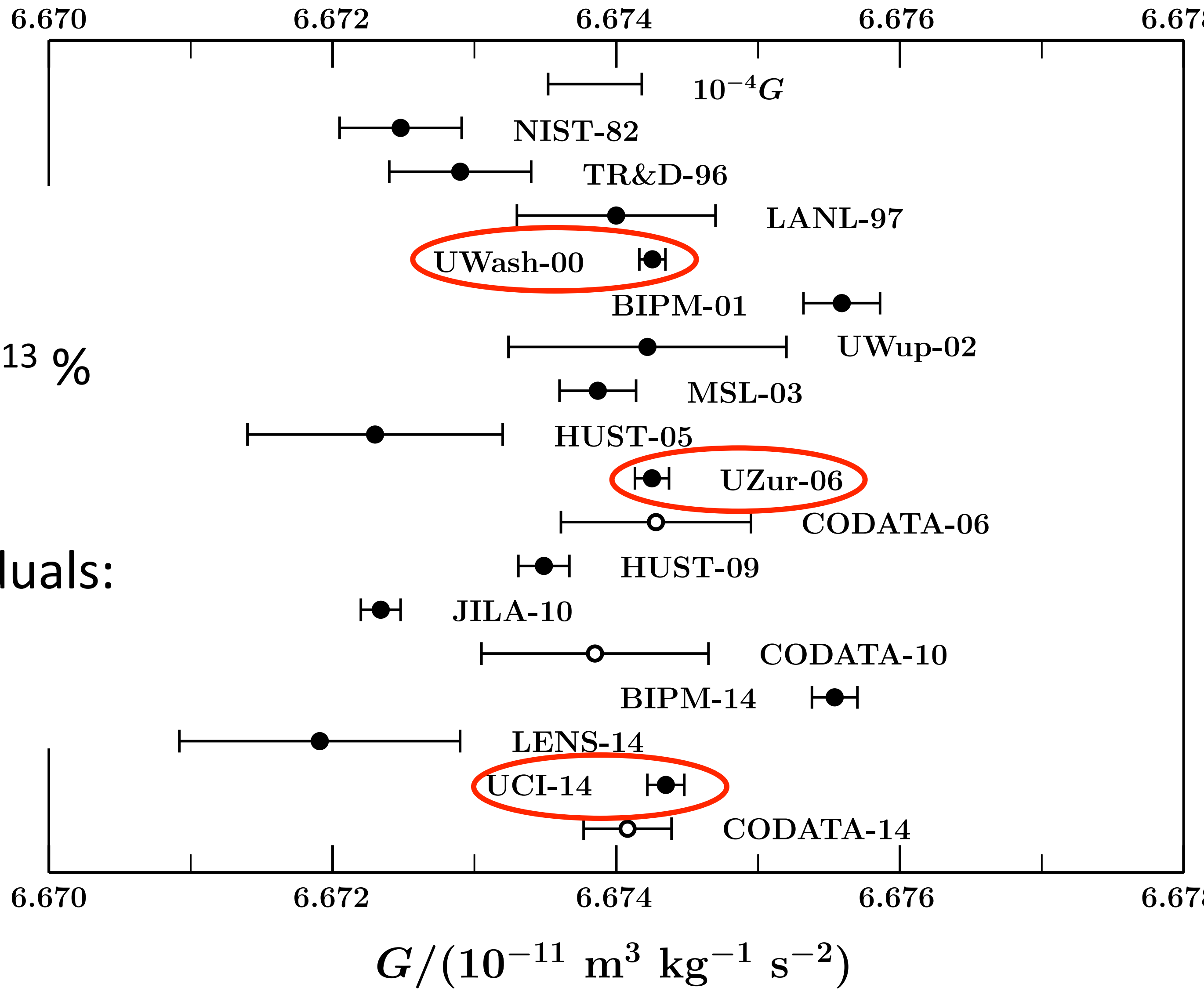
χ^2: 318

DOF: 13

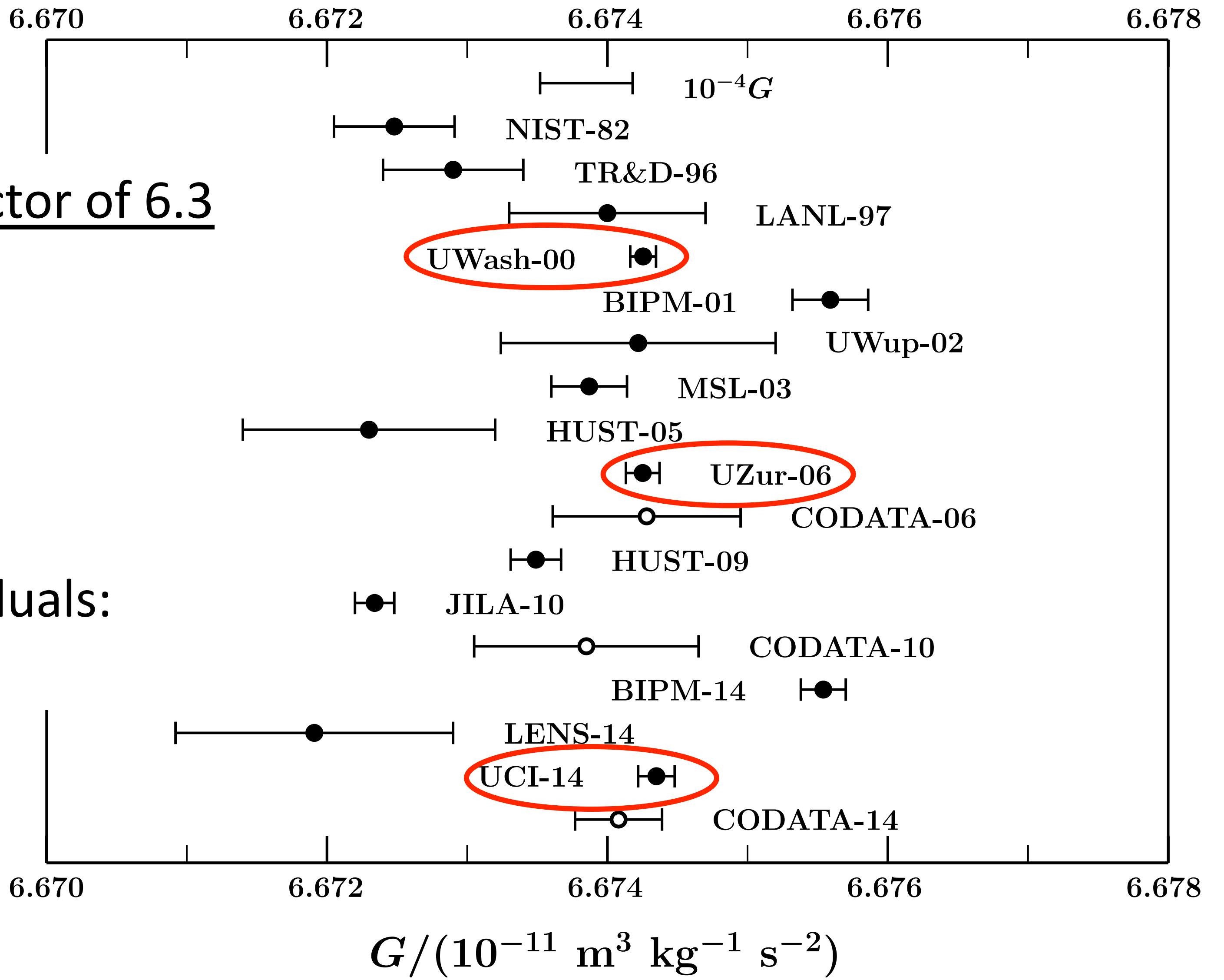
Prob. χ^2: 6.8×10^{-13} %

R_B: 4.95

Max. reduced residuals:
-12.4, 9.14



$$G = 6.67408(31) \times 10^{-11}\ \mathrm{m^3\ kg^{-1}\ s^{-2}}$$
$$[4.7 \times 10^{-5}]$$



With expansion factor of 6.3

χ^2: 8.05

DOF: 13

Prob. χ^2: 84%

R_B: 0.79

Max. reduced residuals:

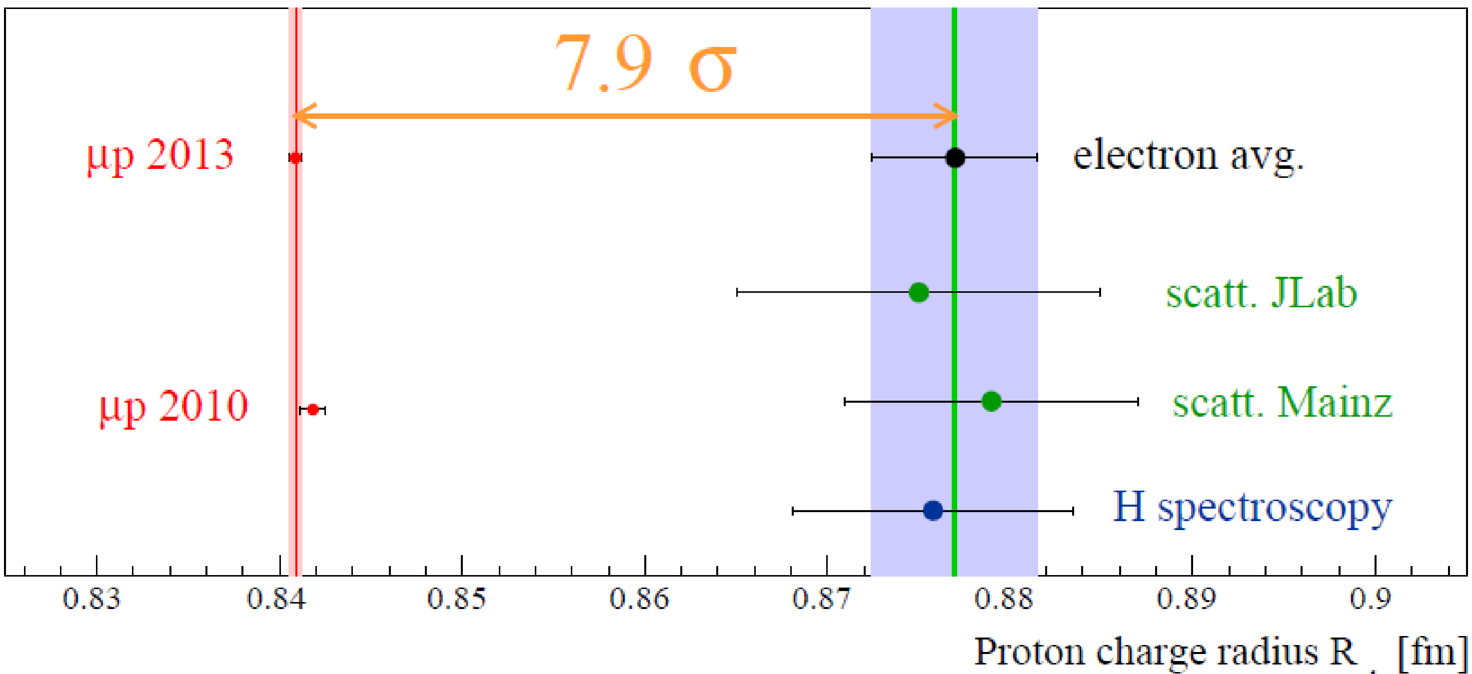
-1.98, 1.44

Rydberg constant, muonic hydrogen, and the proton radius

The proton rms charge radius measured with

electrons: 0.8770 ± 0.0045 fm

muons: 0.8409 ± 0.0004 fm



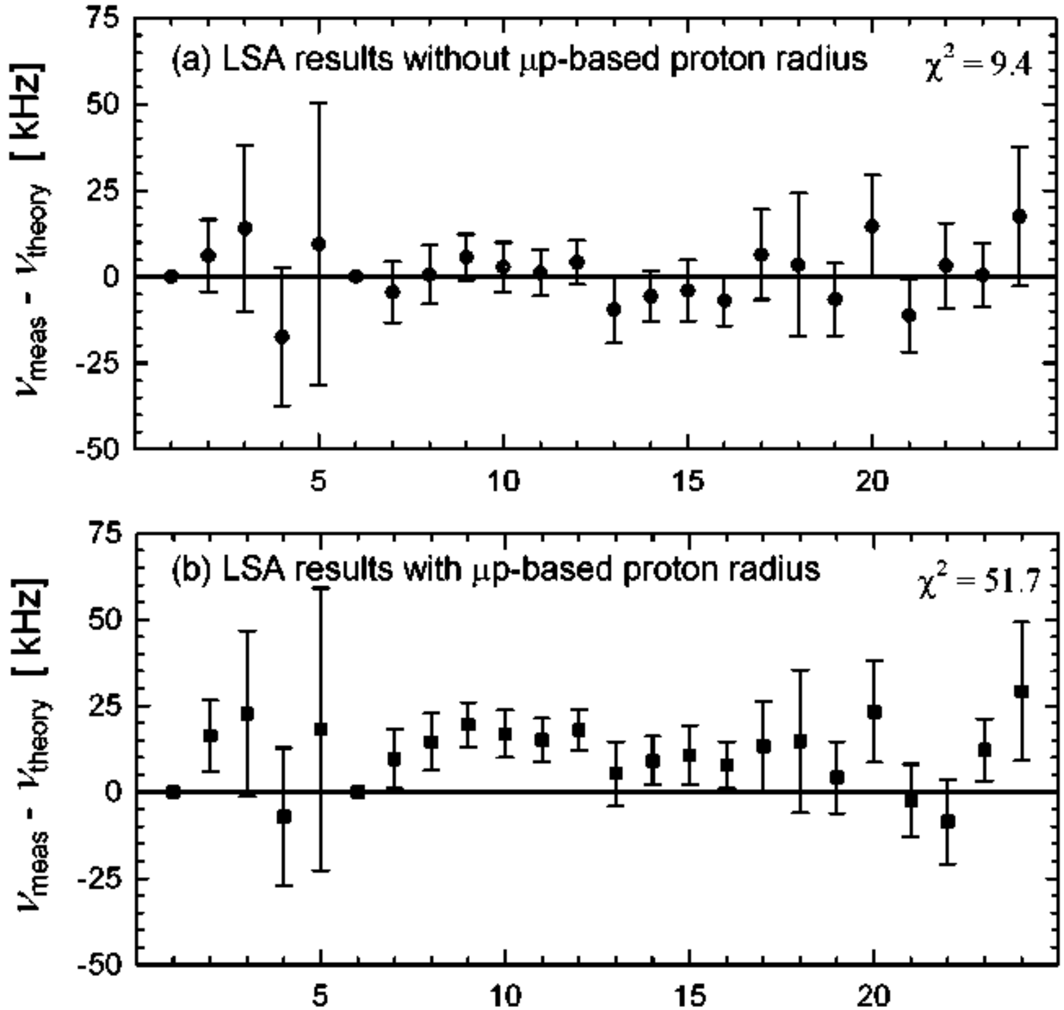
RP, Gilman, Miller, Pachucki, Annu. Rev. Nucl. Part. Sci. 63, 175 (2013).

Input data related to the 2010 CODATA TGFC determination of the Rydberg constant

Transition frequencies in hydrogen and deuterium (experiment – theory)

experiment theory

$$\nu_{\mathrm{H}}\left(1\mathrm{S}_{1/2}-2\mathrm{S}_{1/2}\right)=\frac{3}{4}R_{\infty}c\left[1-\frac{m_{\mathrm{e}}}{m_{\mathrm{p}}}+\frac{11}{48}\alpha^{2}-\frac{28}{9}\frac{\alpha^{3}}{\pi}\ln\alpha^{-2}-\frac{14}{9}\left(\frac{\alpha R_{\mathrm{p}}}{ƛ_{\mathrm{C}}}\right)^{2}+\ldots\right.$$



CODATA TGFC meeting 1 – 2 November, 2014

Outline

- Past adjustments of the constants
- Role and methodology of CODATA TGFC
- 2014 Least Squares Adjustment
- **CODATA and the new SI**

New SI

(http://www.bipm.org/en/measurement-units/new-si/)

Future revision of the SI | What? | Why? | When? | Ongoing work | Communication and debate; draft documents | FAQs; More info.

The New SI based on fixed values of:

- Planck constant, h
- Avogadro constant, N_A
- elementary charge, e
- Boltzmann constant, k

Resolution 1 of the 24th meeting of the CGPM:

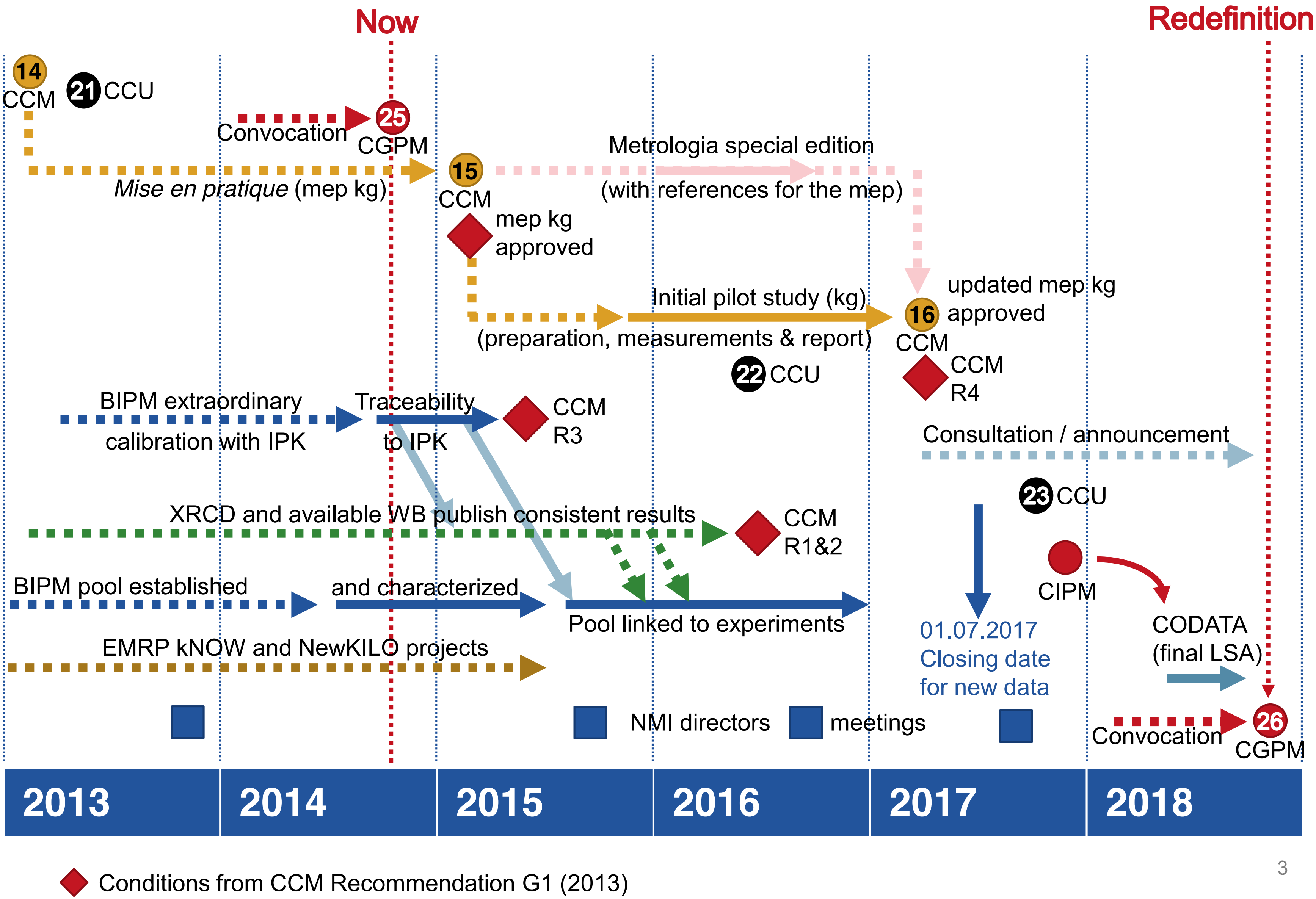
Invites:

- CODATA to continue to provide adjusted values of the fundamental physical constants . . . *since these CODATA values and uncertainties will be those used for the revised SI*

- SI road-map (updated 2014)
- Resolution 1 of the CGPM (2014): On the future revision of the International System of Units, the SI
- Resolution 1 of the CGPM (2011): On the possible future revision of the International System of Units, the SI

On the road to redefinition

Joint CCM and CCU roadmap for the new SI



Critical Deadlines

1 July 2017

Closing date for data for special CODATA constants adjustment to determine exact values of *h*, *e*, *k*, and N_A for 2018 revised SI (International System of Units).

BY this date data must be published or available in a preprint <u>accepted</u> for publication.

Critical Deadlines

1 July 2018

Closing date for data for CODATA constants adjustment to determine new set of CODATA recommended values consistent with the revised SI (*replaces 31 December 2018 normal closing date*).

By this date data should be published or available in a preprint for publication.

Summary

- **In any determination of the best values and uncertainties of parameters (i.e. constants), input data must be fully investigated before any analysis**

- **Significant progress of the input data that determine the constants that will be define the new SI (h, e, N_a, k)**