Physikalisch-Technische Bundesanstalt
Braunschweig und Berlin
Nationales Metrologieinstitut

X-ray Crystal Density Method to Determine the Avogadro and Planck Constants

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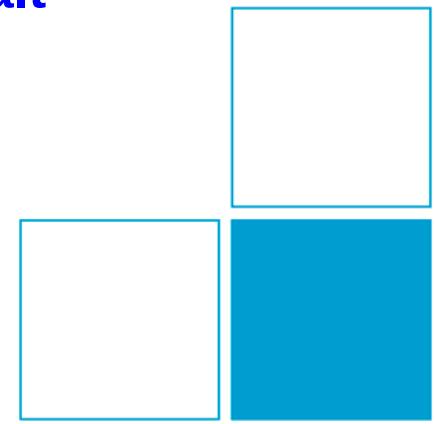


Proposed New Definition of the Kilogram

The kilogram, symbol kg, is the SI unit of mass. It is defined by taking the fixed numerical value of the Planck constant h to be 6.626 070 040 x 10^{-34} when expressed in the unit J s, which is equal to kg m^2 s^{-1}, where the metre and the second are defined in terms of c and $\Delta\nu_{Cs}$.

*) X represents one or more digits to be added at the time the new definition is finally adopted.

$$N_A h = \frac{\alpha^2 M(e^-) c}{2 R_\infty}$$

$N_A h$ = 3.990 312 7110(18) × 10^{-10} Js/mol,
with relative uncertainty of **0.45 × 10^{-9}**

Amedeo Avogadro
(1776-1856)

Max Planck
(1858-1947)

Avogadro Constant

Definition of Avogadro constant N_A

- Number of molecules per mol
- $6.022... \times 10^{23}$ mol^{-1}

Amedeo Avogadro
(1776-1856)

Current definition of mol

- Number "entities" like ^{12}C atoms in 12 g
- i. e. $6.022... \times 10^{23}$ ^{12}C atoms have a mass of 12 g

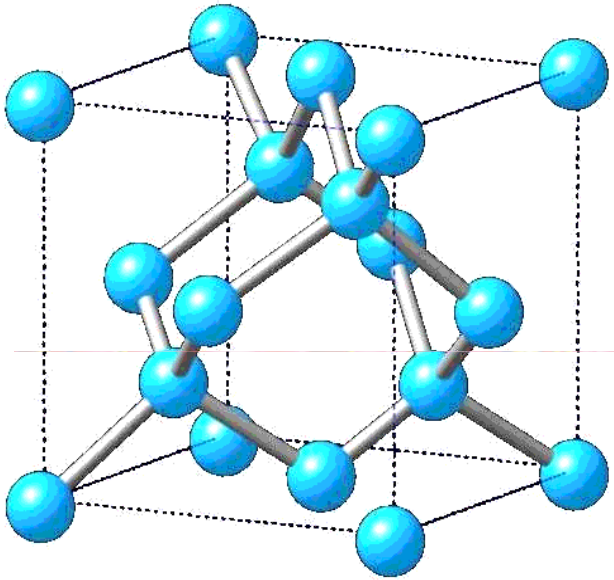
$$12 \text{ g/mol} = N_A \, m(^{12}\text{C})$$

Faraday constant $F = N_A \, e$ (e: elementary charge)

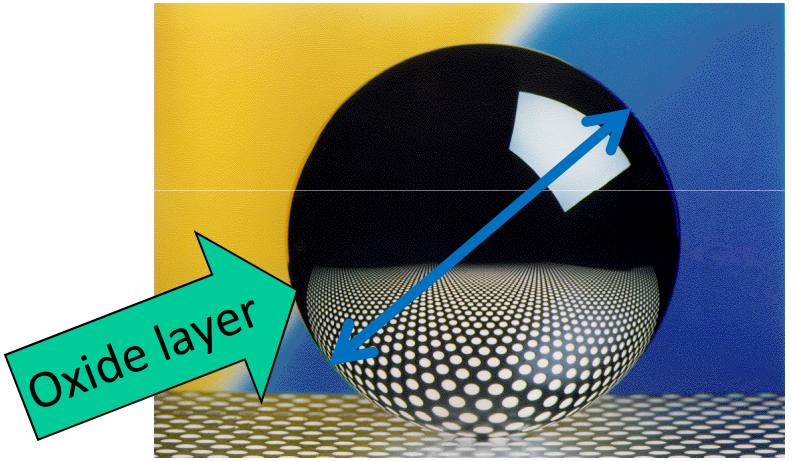
Molar gas constant $R = N_A \, k$ (k: Boltzmann constant)

Counting Atoms: XRCD Method

Use of a silicon crystal!

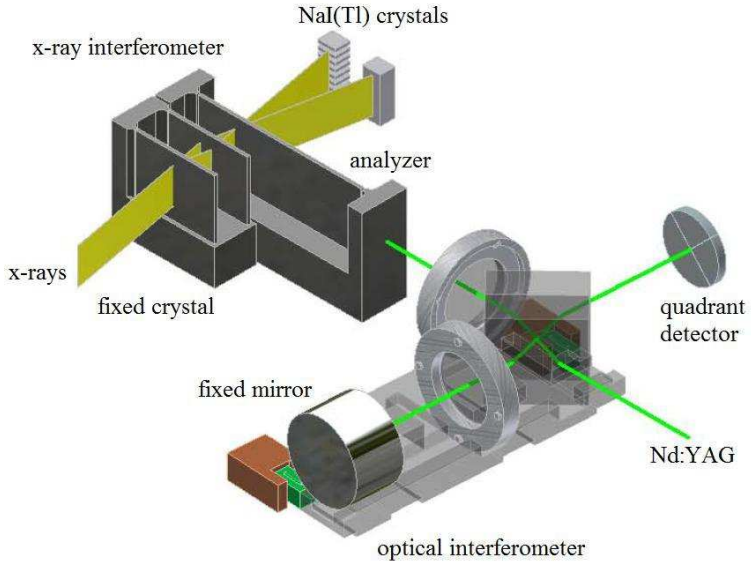


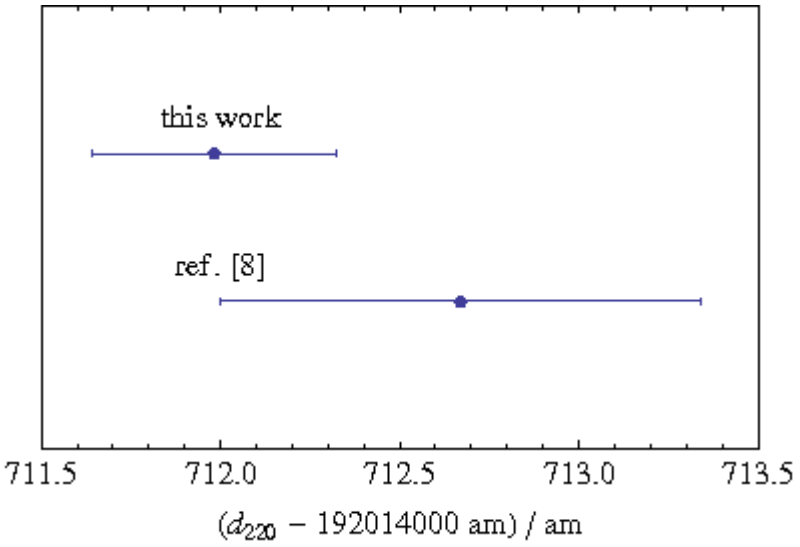
1. Volume a_0^3 of the unit cell
2. Volume of an atom: $a_0^3/8$
3. Volume V of a sphere
4. Number N of the atoms



$$N_A = \frac{8V}{a_0^3} \cdot \frac{M_{mol}}{m_{sphere}}$$

Lattice parameter measurement (INRIM)



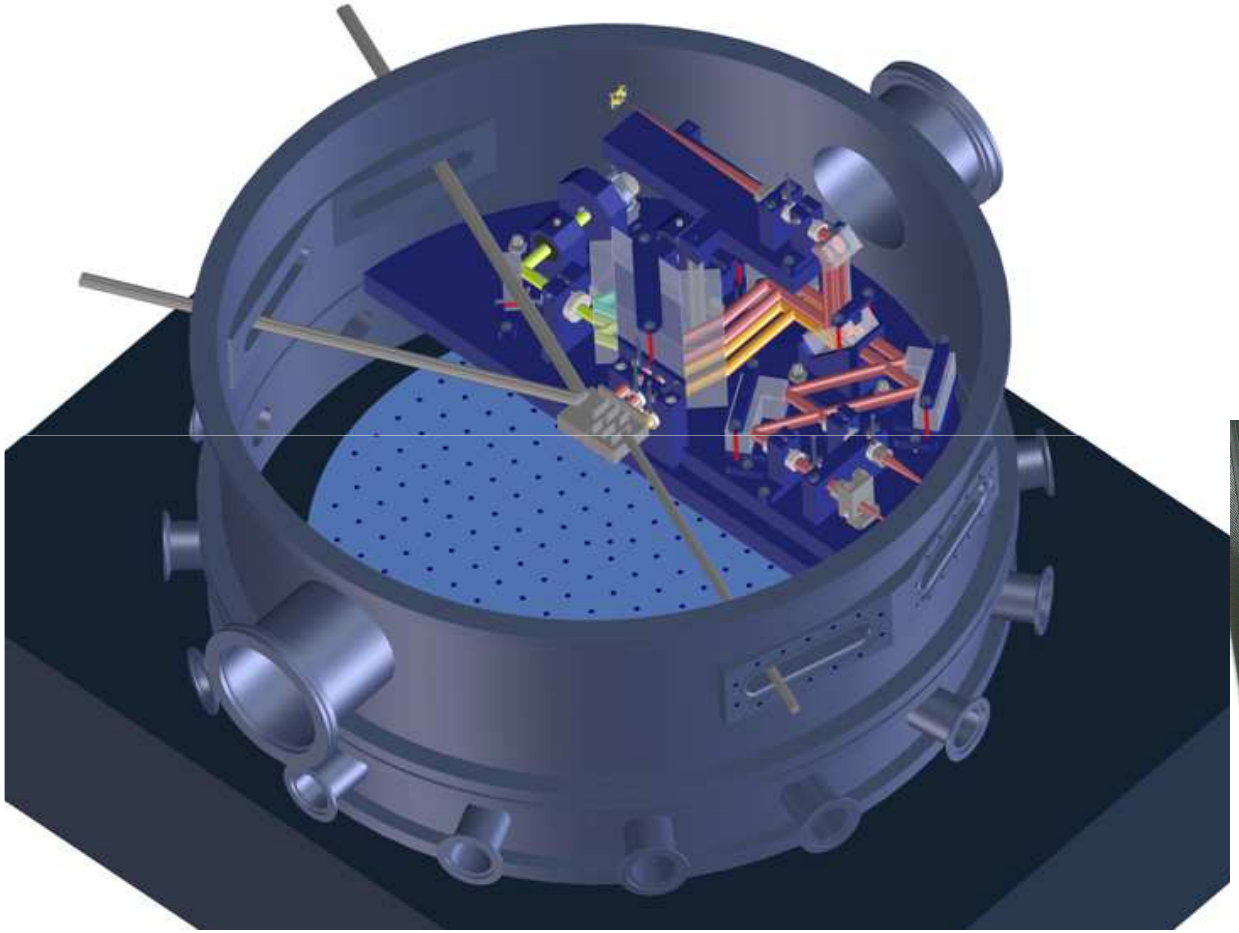


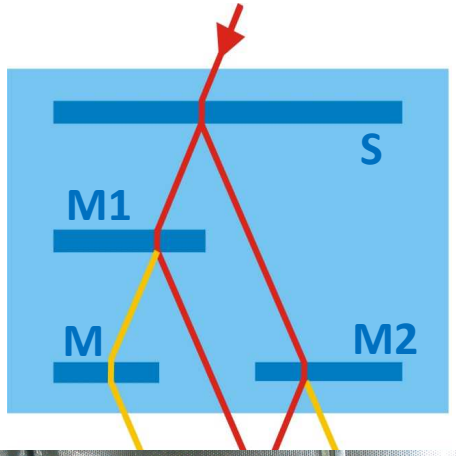
d_{220}(2011)=192014712.67(67) am

d_{220}(2014)=192014711.98(34) am

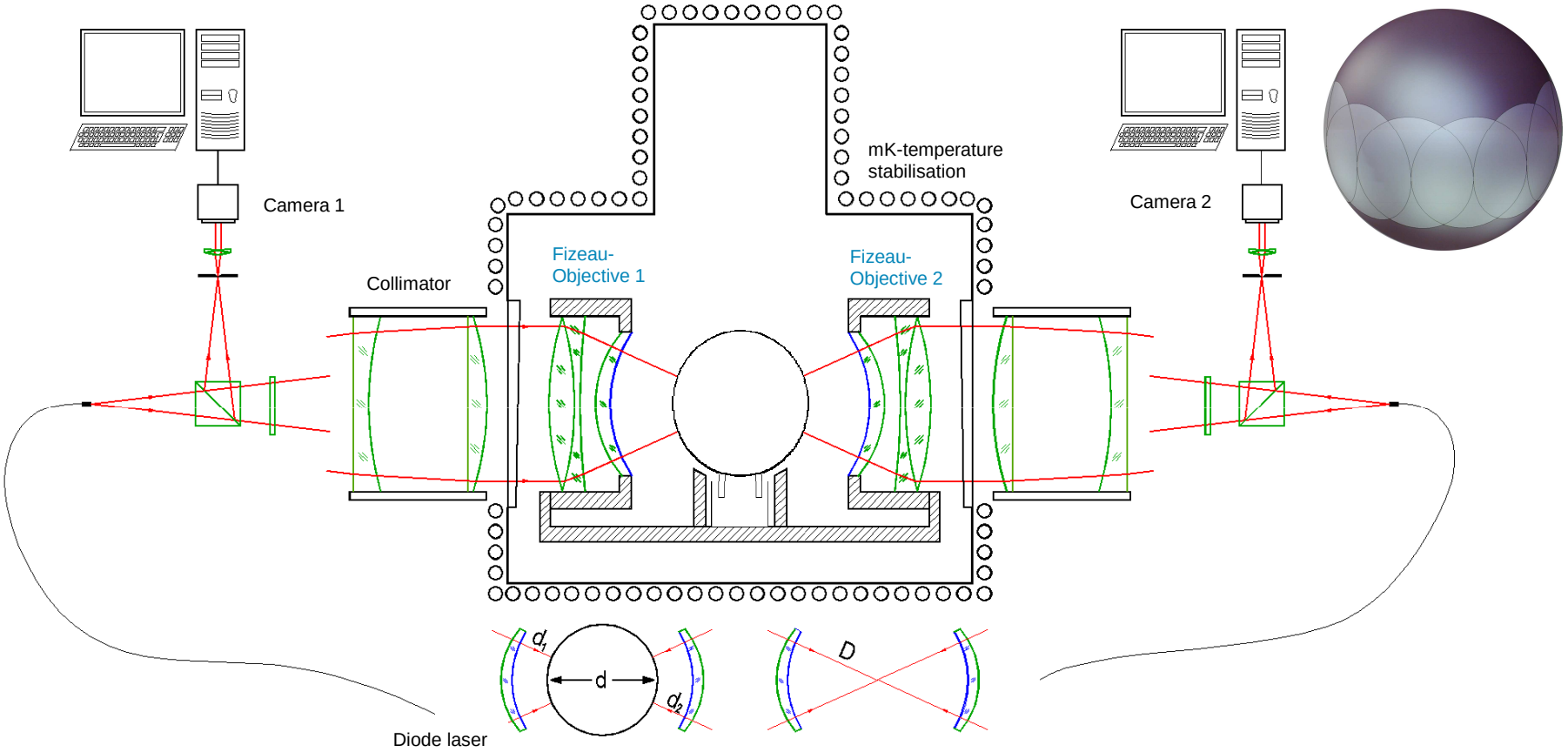
u_r(2014) = 1.8 x 10^{-9}

Lattice parameter set-up at PTB





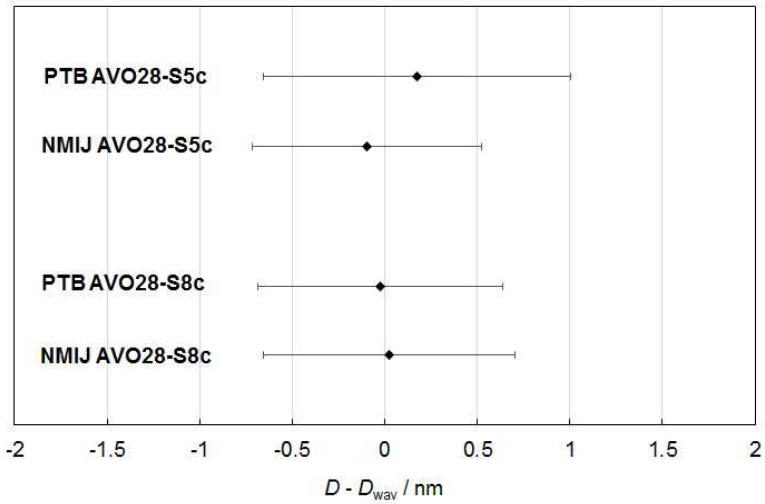
Sphere Interferometer of PTB



$d = D - d_1 - d_2$

Diameter results (2014)

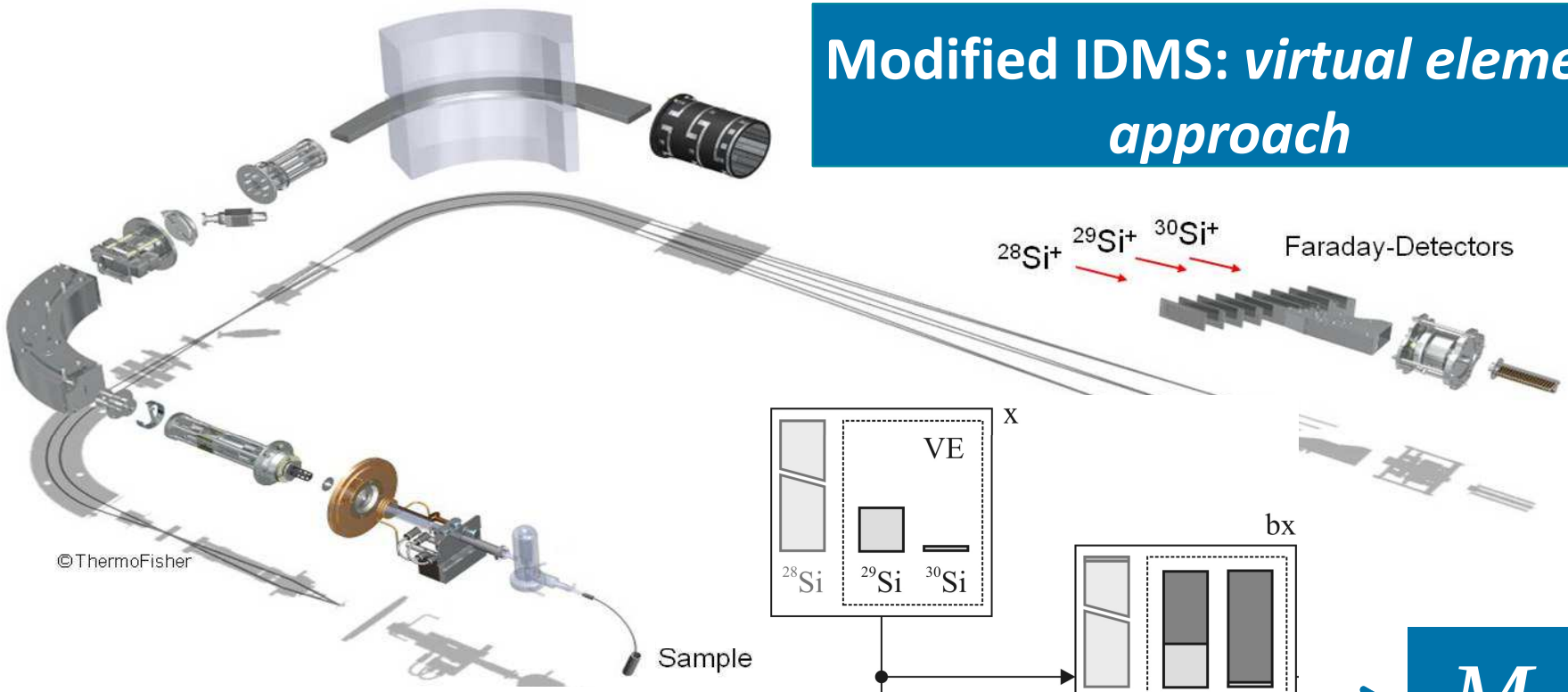
Sphere	Lab.	Mean apparent diameter/nm	Relative Uncertainty in 10^{-9}
AVO28-S5c	PTB	93 710 811.38(83)	9
AVO28-S5c	NMIJ	93 710 811.11(62)	7
AVO28-S5c	weighted mean	93 710 811.21(50)	5
AVO28-S8c	PTB	93 701 526.24(66)	7
AVO28-S8c	NMIJ	93 701 526.29(68)	7
AVO28-S8c	weighted mean	93 701 526.26(47)	5



$$u(\text{volume}) = 1.5 \times 10^{-8}\, V$$

Molar Mass Determination

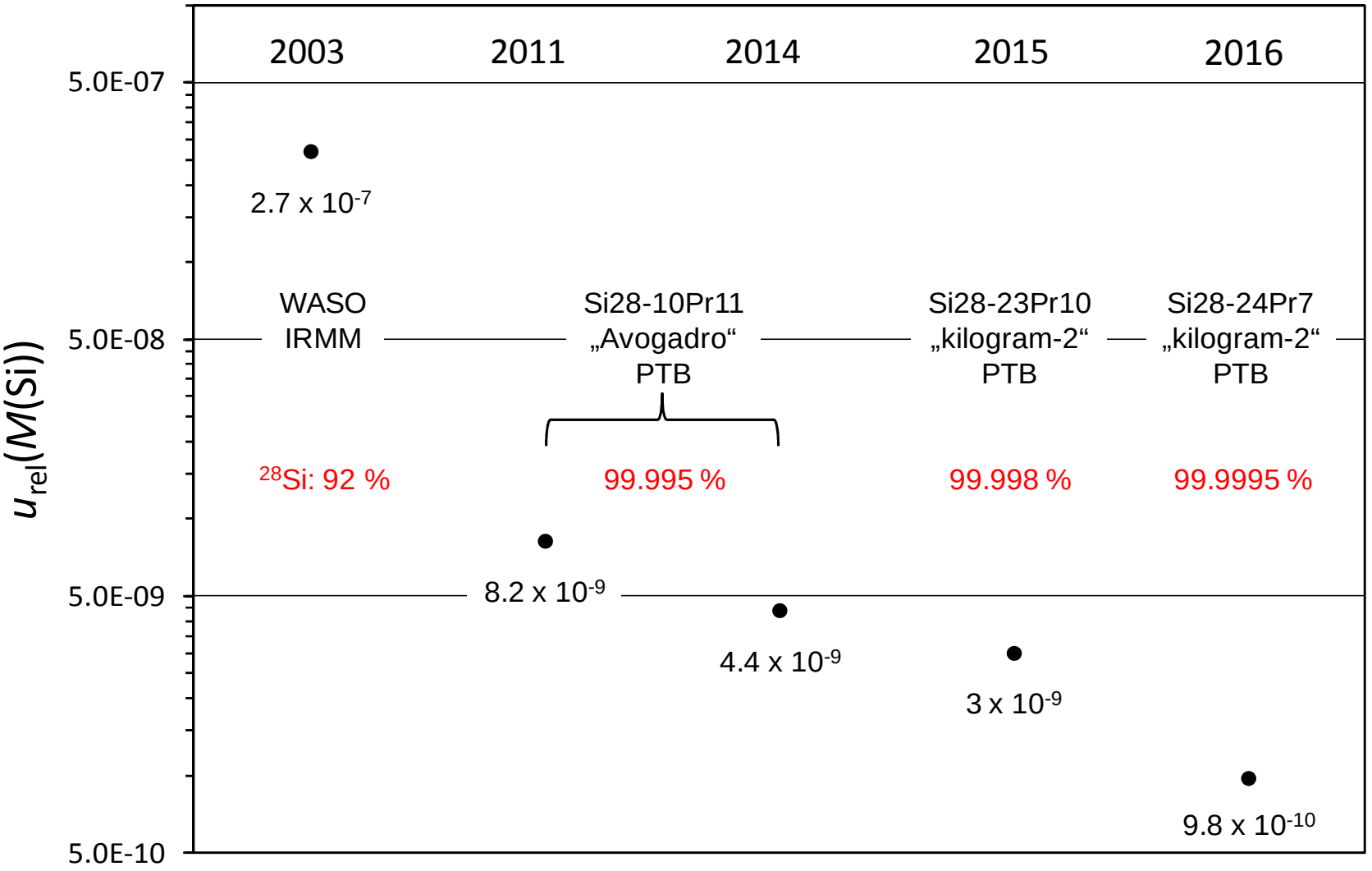
Modified IDMS: *virtual element approach*



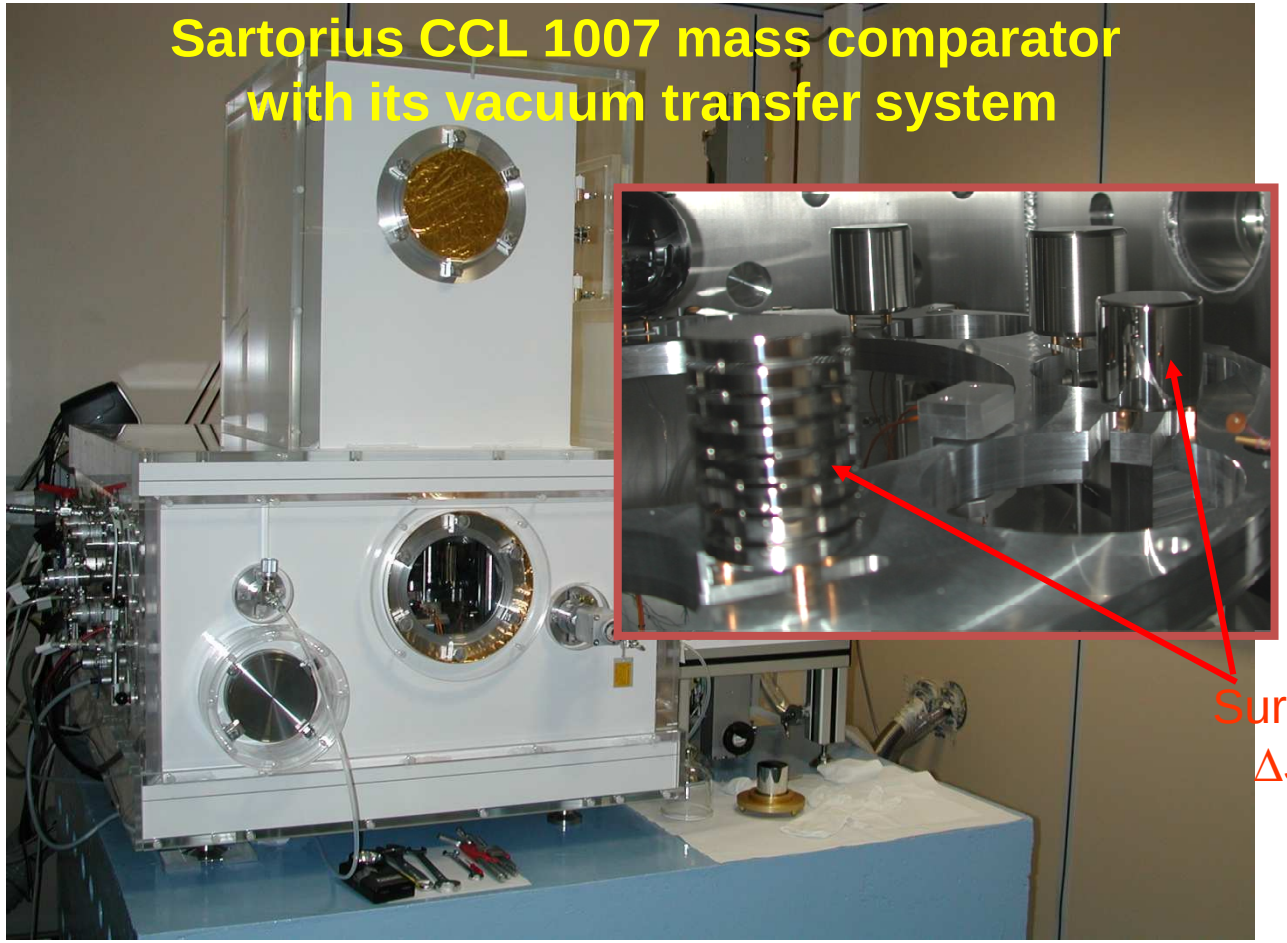
- Three samples: ^{28}Si-material („*x*“)
  ^{30}Si-enriched („*y*“)
  IDMS-blend („*bx*“)
- $R(^{30}Si/^{29}Si)$ measured in *x*, *y*, *bx*

A. Pramann et al.
Metrologia 48 (2011) S20-S25

Molar Mass Uncertainty

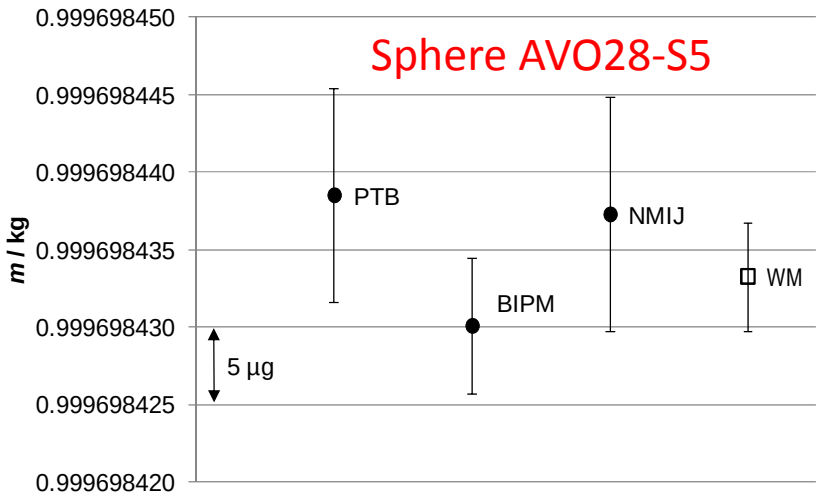


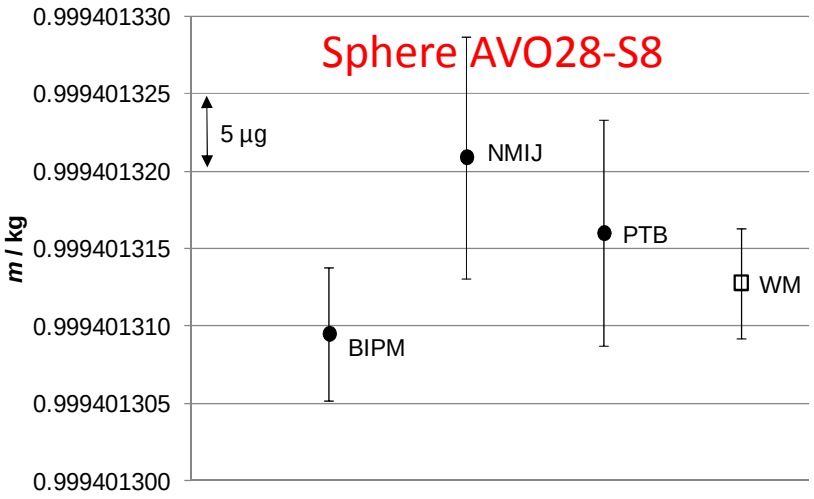
Mass Determination (at BIPM)



Mass measurements

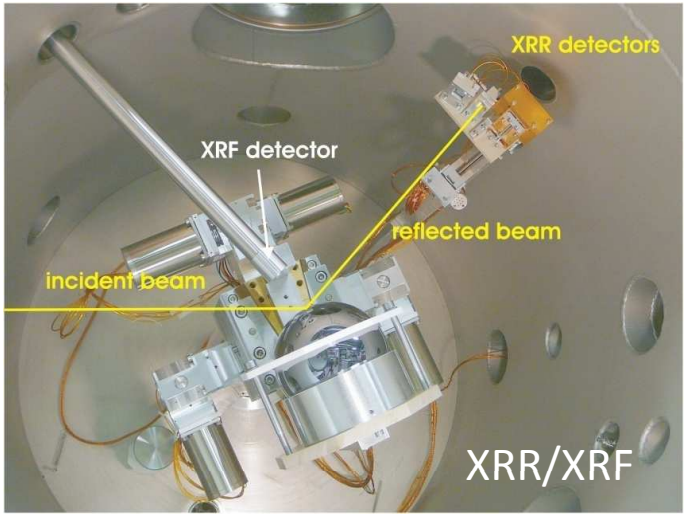
- Extraordinary calibrations using the IPK
- Uncertainty of the weighted mean: 3.5 µg

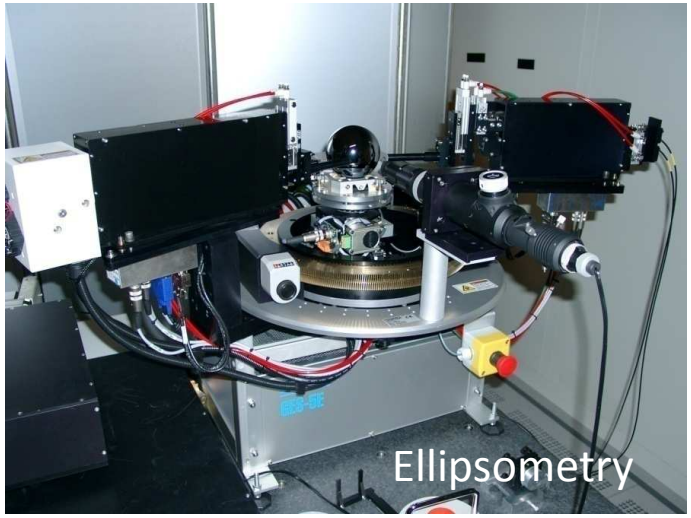




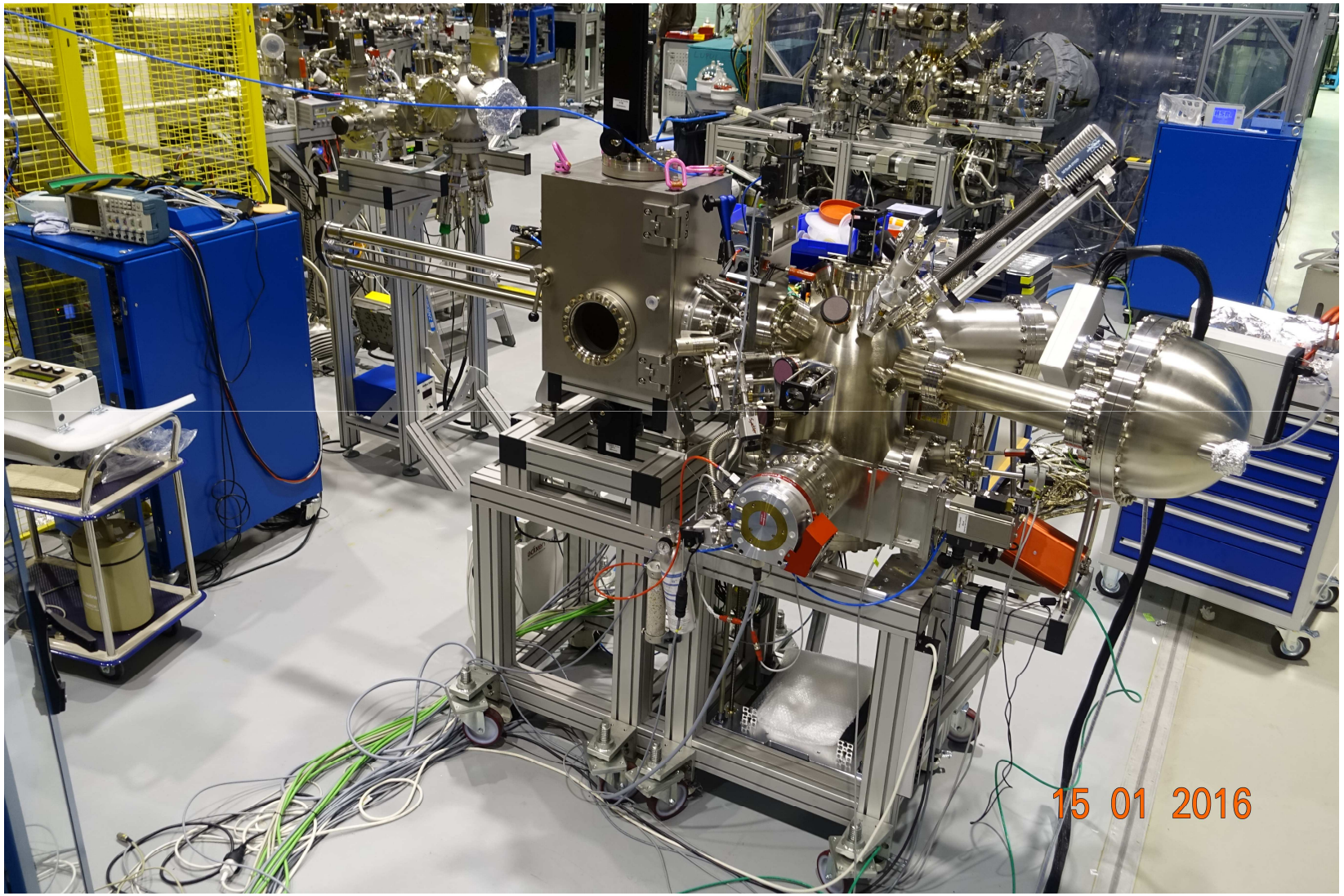
Surface Characterisation

Surface	Mass	Method
Carbon	15 µg	XRF, XPS, IR
Water	8 µg	Gravimetric
Si oxide	70 µg	XPS, XRF, XRR, SE
Metals	< 1 µg	XRF
Si crystal		





Surface layer measurement: XPS/XRF

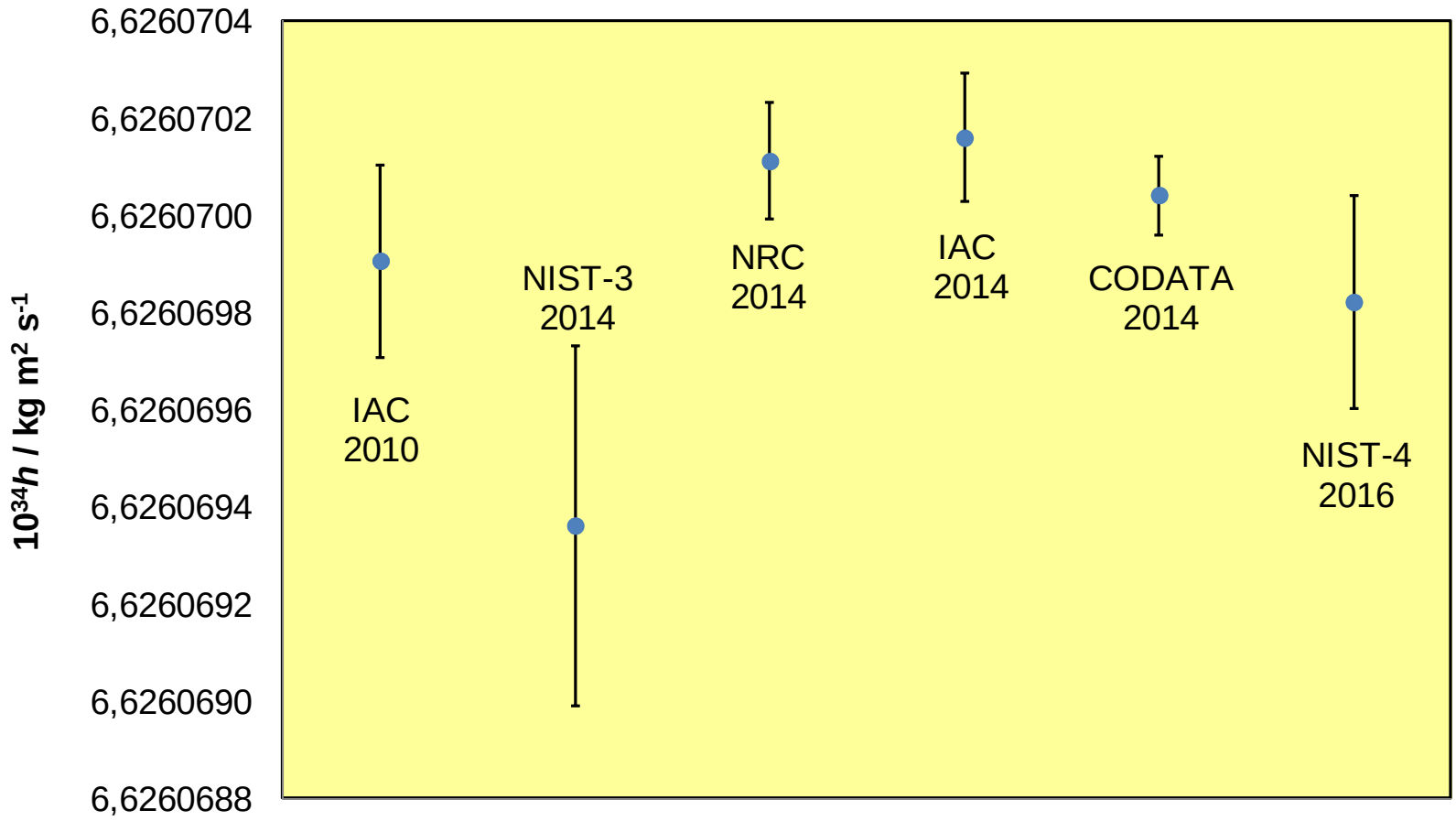


Uncertainty budget (2014)

Only one sphere (AVO28-S5c):

Quantity	Relative uncertainty/10^{-9}	Contribution/%
Molar mass	5	6
Lattice parameter	5	6
Surface	10	23
Sphere volume	16	59
Sphere mass	4	4
Point defects	3	2
Total	21	100

Values of the Planck Constant (2016)



Improvements until June 2017

Aim: Avogadro value with relative uncertainty below 1.5×10^{-8}

Improvements:

a) **New XPS/XRF apparatus for spheres at PTB**

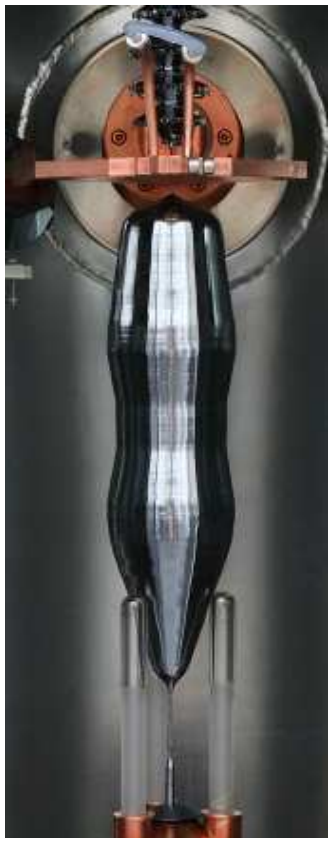
b) **New XPS apparatus for spheres at NMIJ**

c) **Spheres with better roundness (smaller wavefront abberration)**

d) **New lattice parameter measurement at PTB**

e) **Avogadro constant determined using Si-28 with higher enrichment**

Existing Si-28 Single Crystals



AVO28
99.995%

kg-2.1
99.998%

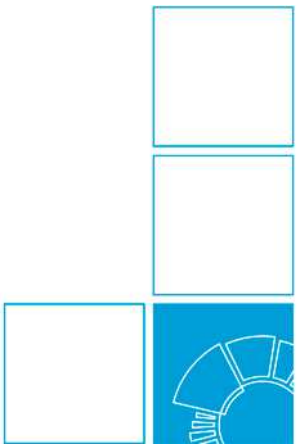
kg-2.2
99.9995%

...

Thank you very much for your attention!

Questions?

Comments?



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