The molar mass of highly enriched silicon:

”Counting” Si atoms in a silicon sphere

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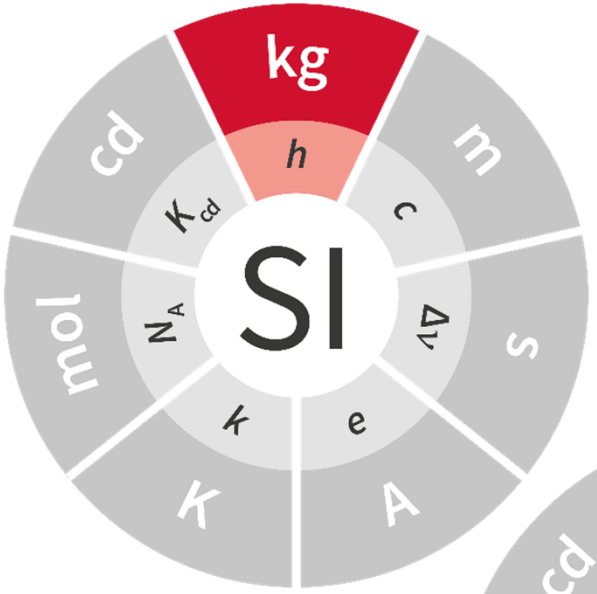
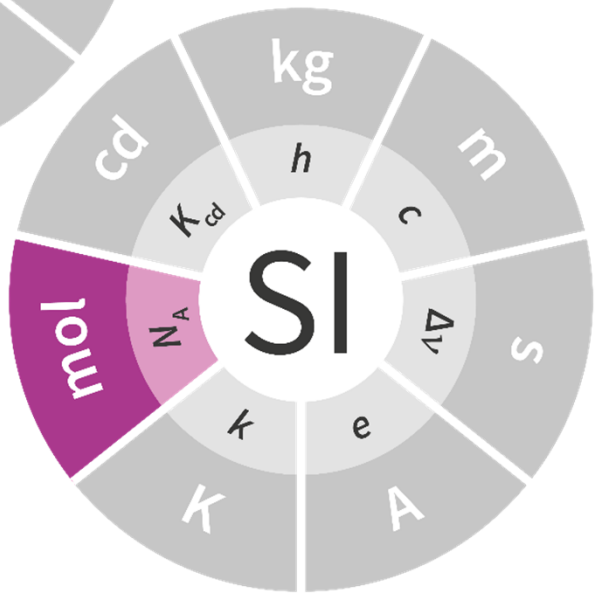
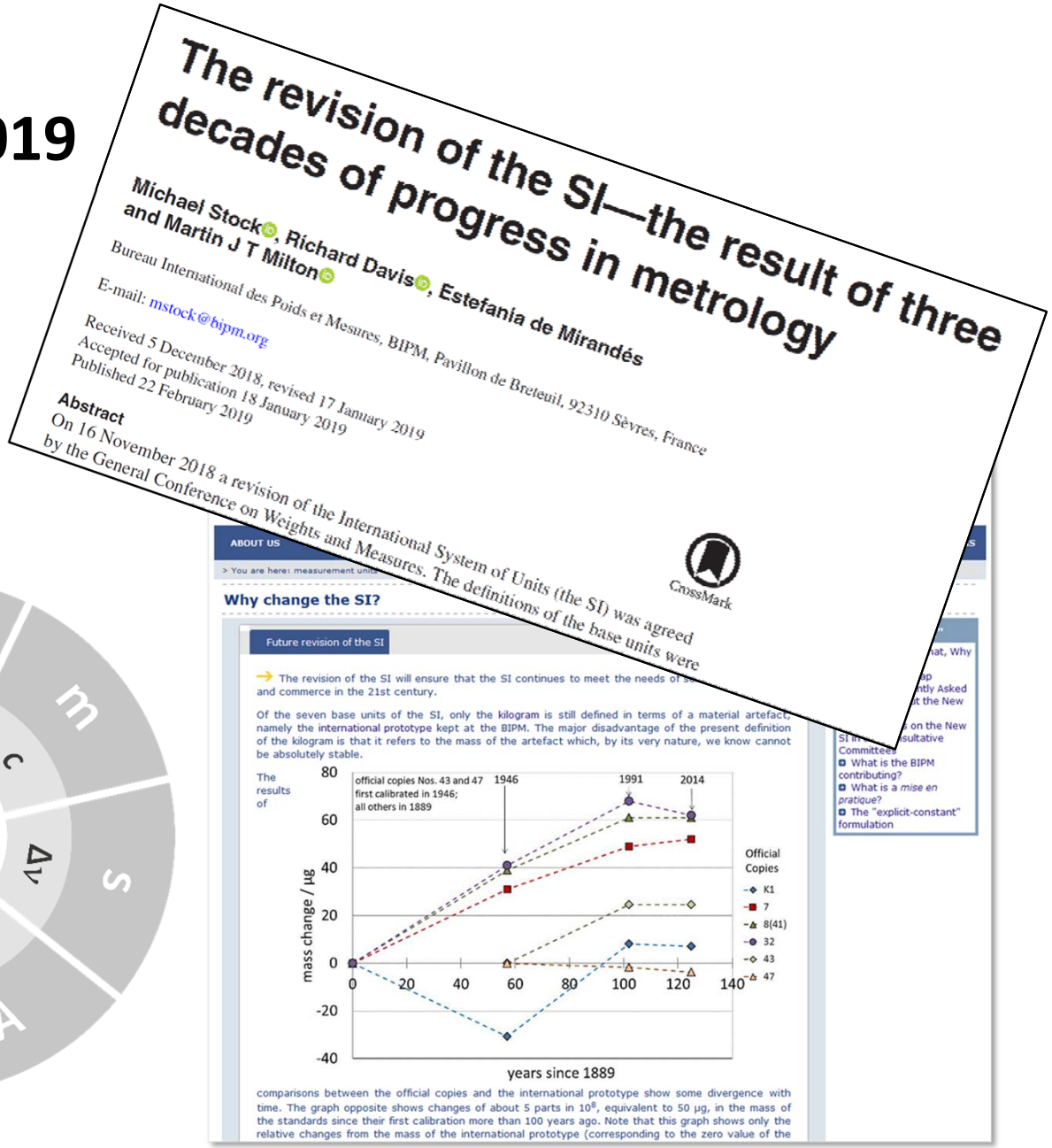
Motivation/background

Revision of the SI in 2019







The revision of the SI—the result of three decades of progress in metrology

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Abstract

On 16 November 2018 a revision of the International System of Units (the SI) was agreed by the General Conference on Weights and Measures. The definitions of the base units were

ABOUT US

> You are here: measurement units

Why change the SI?

Future revision of the SI

The revision of the SI will ensure that the SI continues to meet the needs of sc and commerce in the 21st century.

Of the seven base units of the SI, only the kilogram is still defined in terms of a material artefact, namely the international prototype kept at the BIPM. The major disadvantage of the present definition of the kilogram is that it refers to the mass of the artefact which, by its very nature, we know cannot be absolutely stable.

The results of

comparisons between the official copies and the international prototype show some divergence with time. The graph opposite shows changes of about 5 parts in 10^8, equivalent to 50 µg, in the mass of the standards since their first calibration more than 100 years ago. Note that this graph shows only the relative changes from the mass of the international prototype (corresponding to the zero value of the

Committees

- What is the BIPM contributing?
- What is a *mise en pratique*?
- The "explicit-constant" formulation

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The "Avogadro Project"

Determination of N_A with $u_{rel}(N_A) < 2\times10^{-8}$

$$1\,\mathrm{mol} = \frac{6.02214076\times10^{23}}{N_A}$$

$$1\,\mathrm{kg} = \frac{h}{6.62607015\times10^{-34}}\,\frac{\mathrm{m}^2}{\mathrm{s}}$$

$$h = \frac{cM_u A_r(\mathrm{e})\alpha^2}{2R_\infty N_A}$$

A new ^{28}Si single crystal: counting the atoms for the new kilogram definition

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Abstract
A new single crystal from isotopically enriched silicon was used to determine the Avogadro constant N_A by the x-ray-crystal density method. The new crystal, named Si28-23Pr11, has

→ **x-ray crystal density method (XRCD)**

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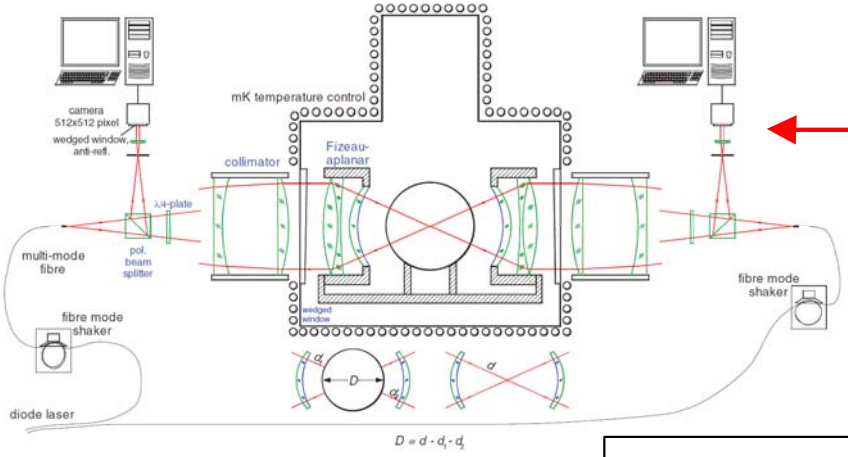
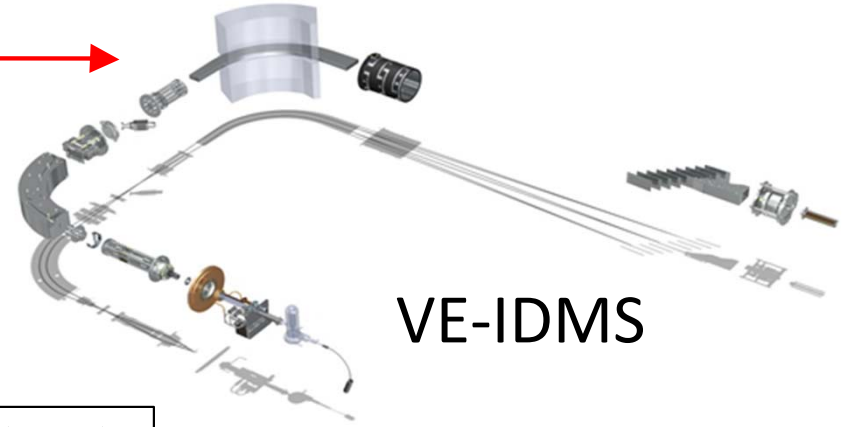
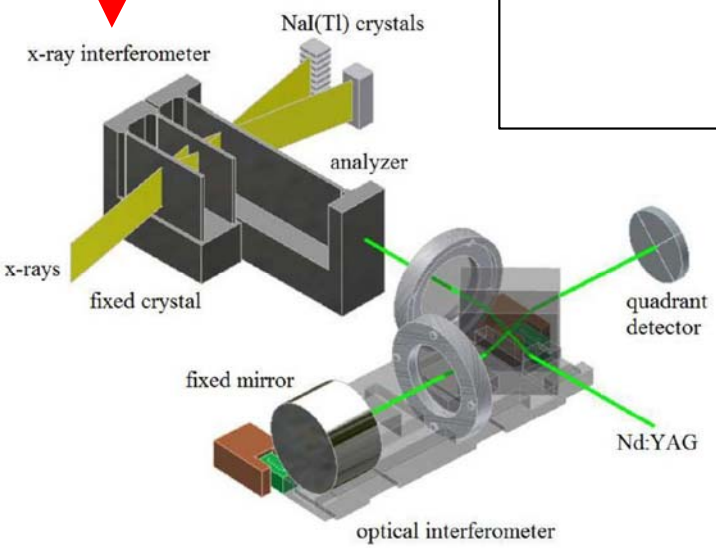
XRCD (I)





VE-IDMS

$$N_A = \underbrace{\frac{8V}{a^3}}_{=N} \underbrace{\frac{M(\mathrm{Si})}{m}}_{=n^{-1}}$$



https://doi.org/ 10.1088/0026-1394/53/5/A19
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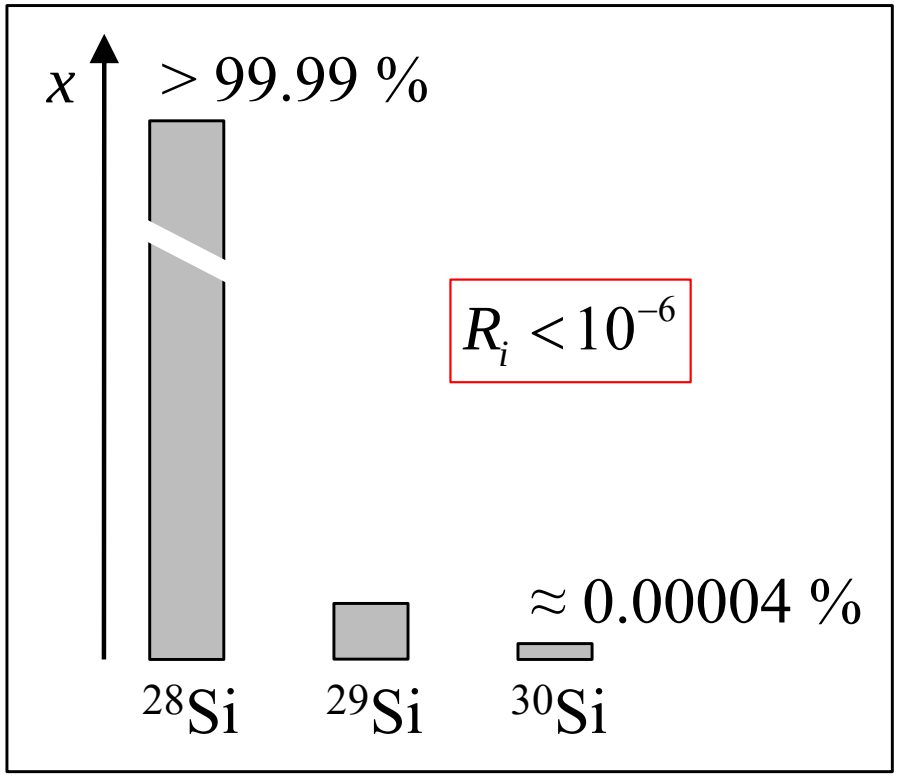
XRCD (II)

Determination of the molar mass of silicon

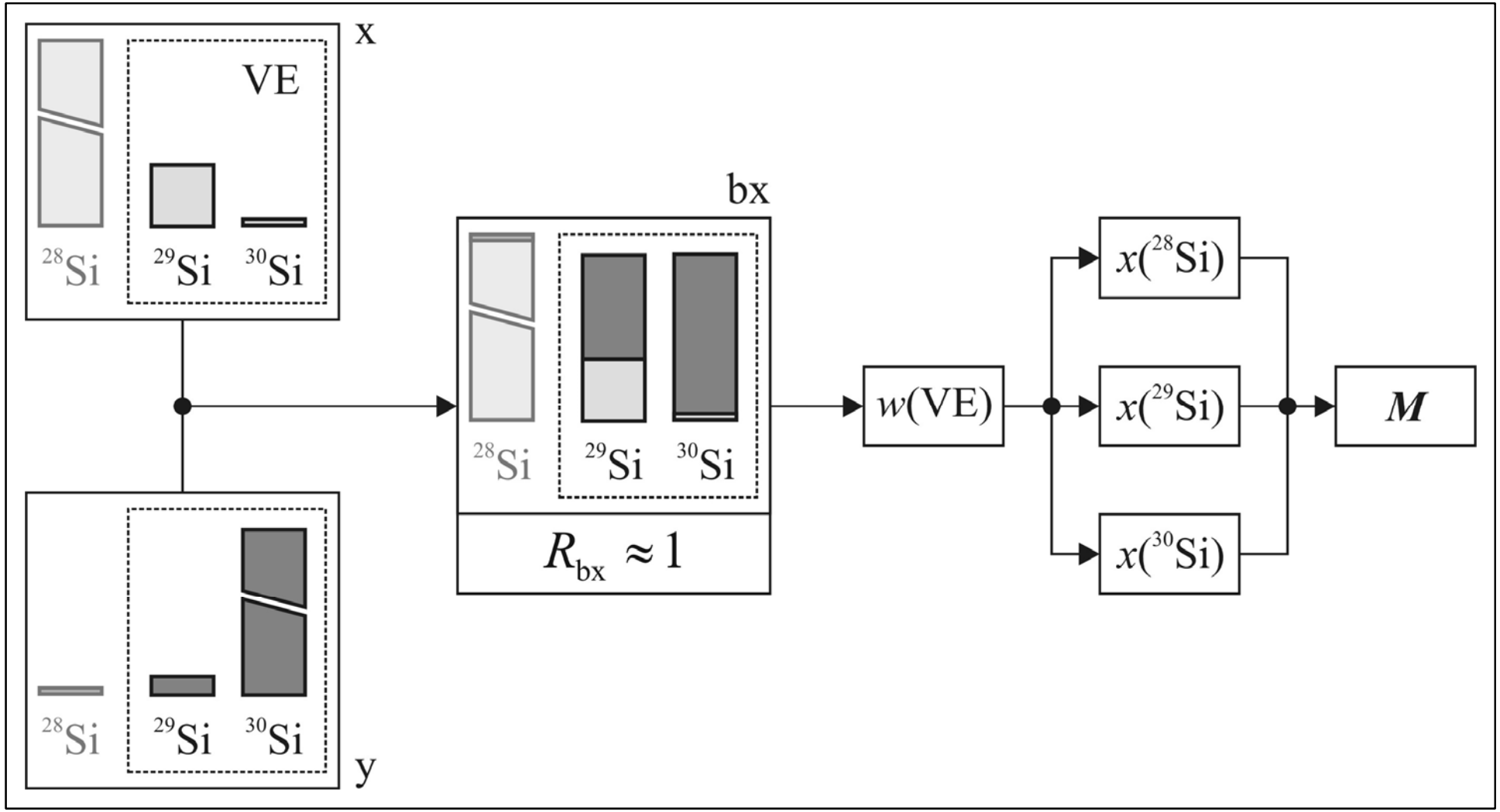
- three isotopes: $^{28}\mathrm{Si}$, $^{29}\mathrm{Si}$, $^{30}\mathrm{Si}$
- amount fractions $x \leftrightarrow$ isotope ratios R

$$M(\mathrm{Si}) = \sum_{i=28}^{30} \left[x\left({}^{i}\mathrm{Si}\right) \times M\left({}^{i}\mathrm{Si}\right) \right]$$

$$x\left({}^{i}\mathrm{Si}\right) = \frac{R_i}{\sum_{j=28}^{30} R_j}$$



Virtual Element IDMS (I)



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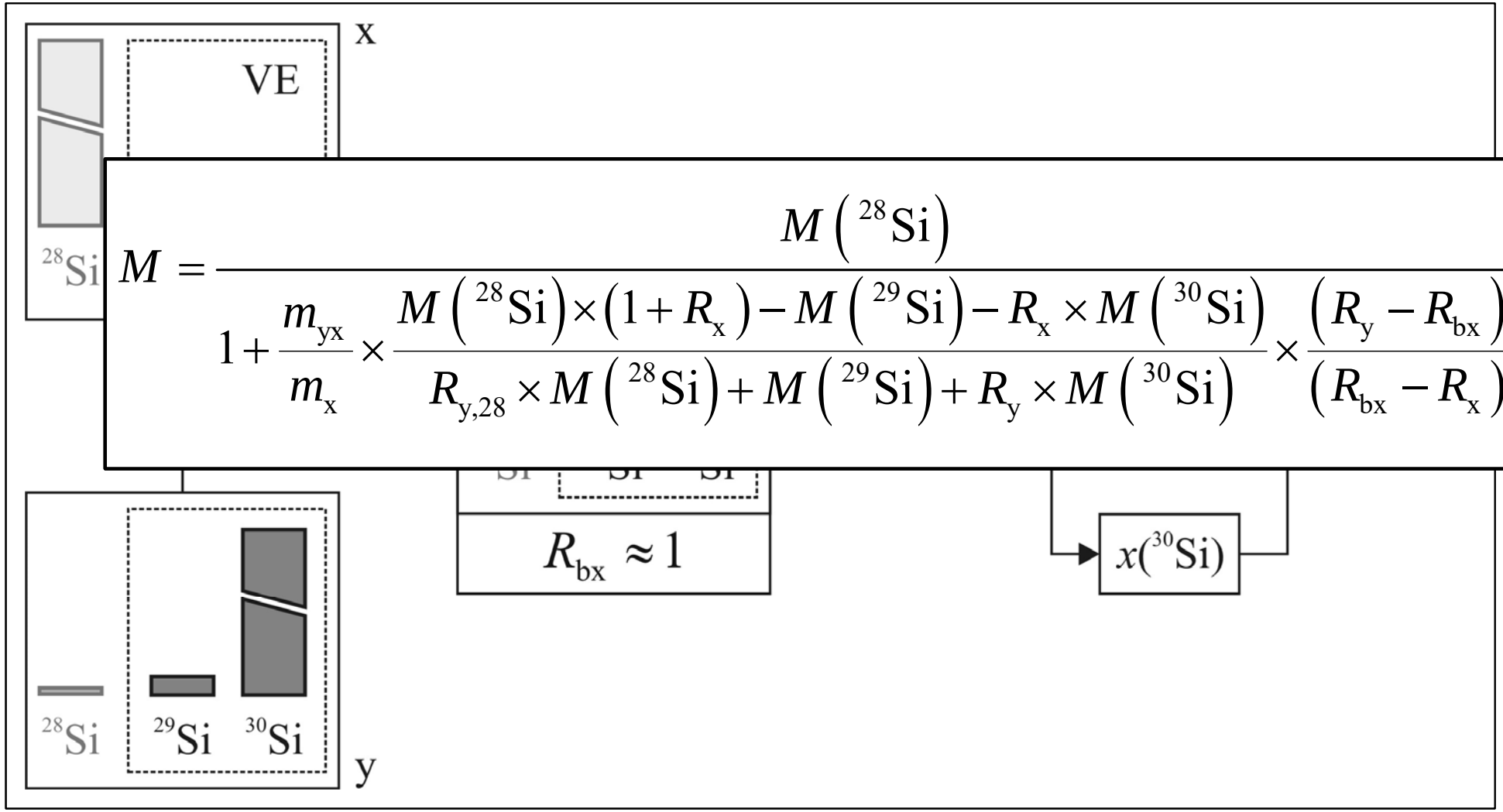
Virtual Element IDMS (I)

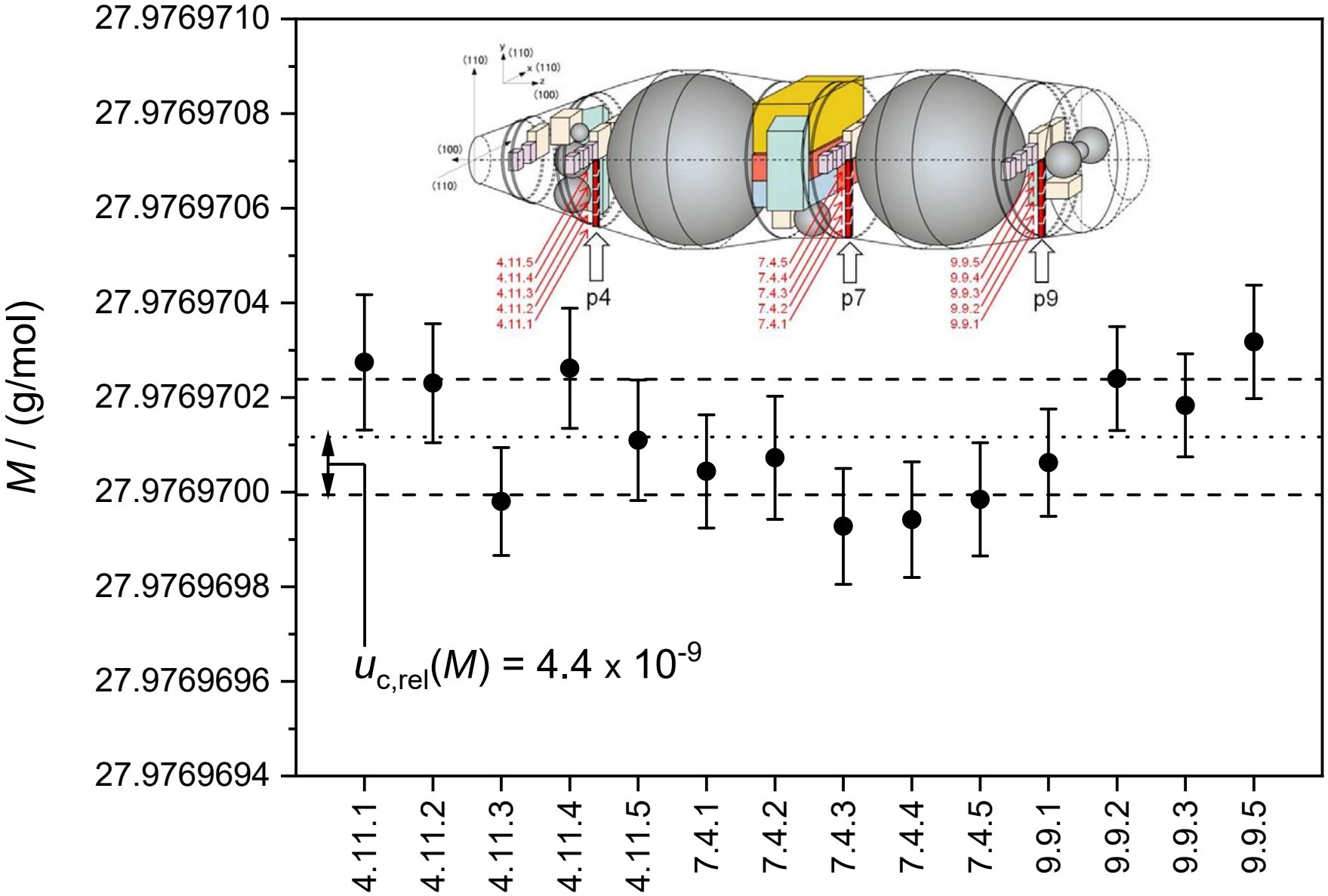


$$M = \frac{M\left(^{28}\mathrm{Si}\right)}{1 + \frac{m_{yx}}{m_x} \times \frac{M\left(^{28}\mathrm{Si}\right) \times \left(1 + R_x\right) - M\left(^{29}\mathrm{Si}\right) - R_x \times M\left(^{30}\mathrm{Si}\right)}{R_{y,28} \times M\left(^{28}\mathrm{Si}\right) + M\left(^{29}\mathrm{Si}\right) + R_y \times M\left(^{30}\mathrm{Si}\right)} \times \frac{\left(R_y - R_{bx}\right)}{\left(R_{bx} - R_x\right)}}$$

Metrologia 47 (2010) 460-463

https://doi.org/10.1088/0026-1394/47/4/012

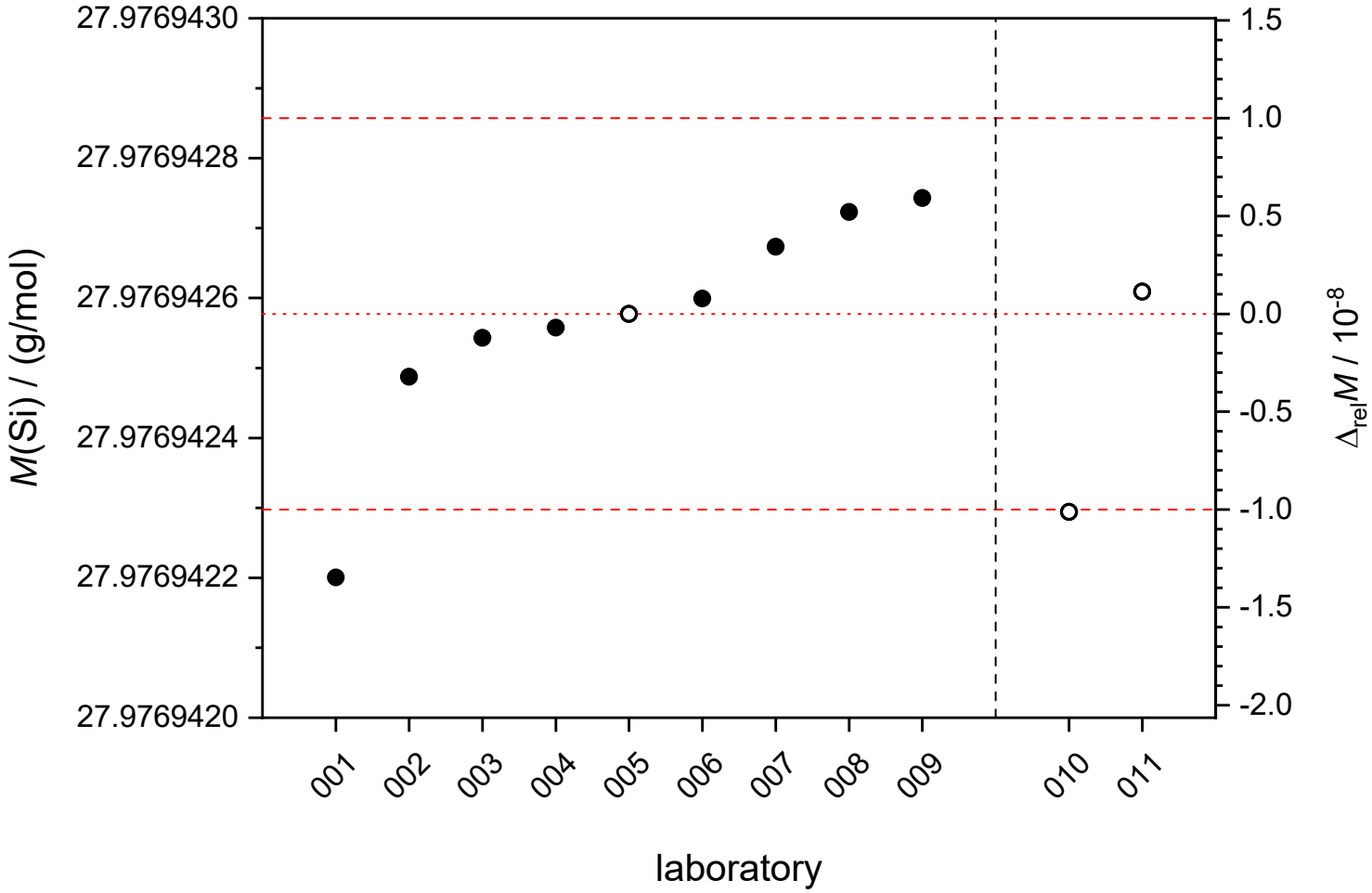
Virtual Element IDMS (II)



https://doi.org/10.1088/0026-1394/52/6/800

Virtual Element IDMS (III)

CCQM-P160 – validation of the novel method



https://doi.org/10.1088/1681-7575/abbdbf

Avogadro constant

XRCD results used for the 2019 revision of the SI

	N_A / (10^{23} × mol^{-1})	$u_{rel}(N_A)$ / 10^{-8}
IAC-11	6.022 140 95(18)	3.0
IAC-15	6.022 140 70(12)	2.0
IAC-17	6.022 140 526(70)	1.2
NMIJ-17	6.022 140 78(15)	2.4

Revision of mol and kg

h = 6.626 070 15 × 10^{-34} J s
N_A = 6.022 140 76 × 10^{23} mol^{-1}

https://doi.org/10.1088/1681-7575/aa950a

Quantities related to counting

Results in elemental and isotope analysis

Quantity	Symbol	Unit
mass fraction	w	kg/kg
isotope ratio	R	mol/mol
amount fraction	x	mol/mol
molar mass	M	kg/mol

Input quantities

Quantity	Symbol	Unit
mass	m	kg
intensity ratio	r	V/V, s^{-1}/s^{-1}

Summary/conclusion

- XRCD as a „counting“ example contributed substantially to the revision of the mole and kg in 2019
- Number of Si atoms in the sphere is equal to the ratio of the volume of the sphere and of a single atom
- Elemental analysis and isotope ratio determination do not require special quantities or units related to counting