redefinition of the mole and the new system of units

zoltan mester

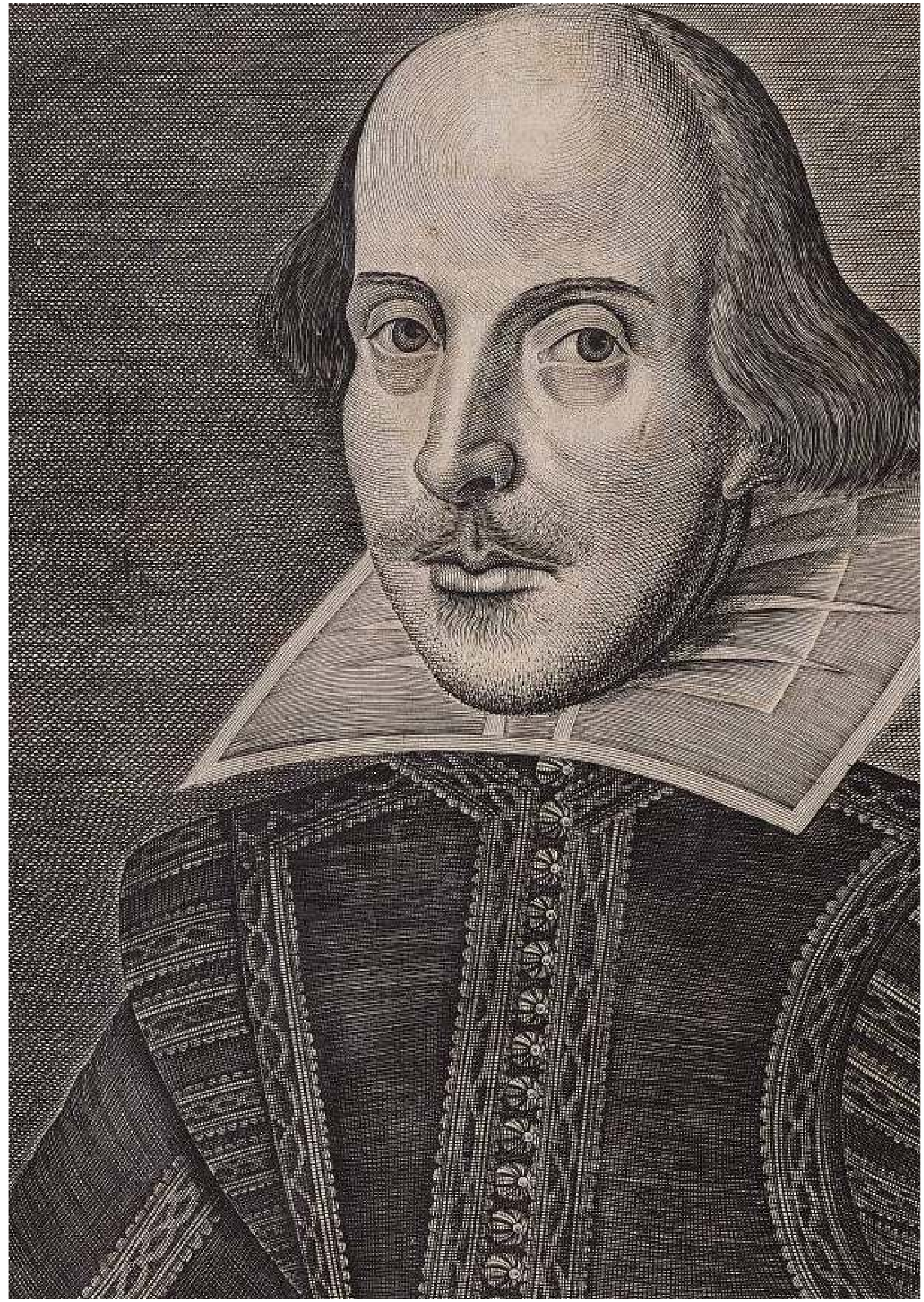
National Research Council Canada
Conseil national de recherches Canada

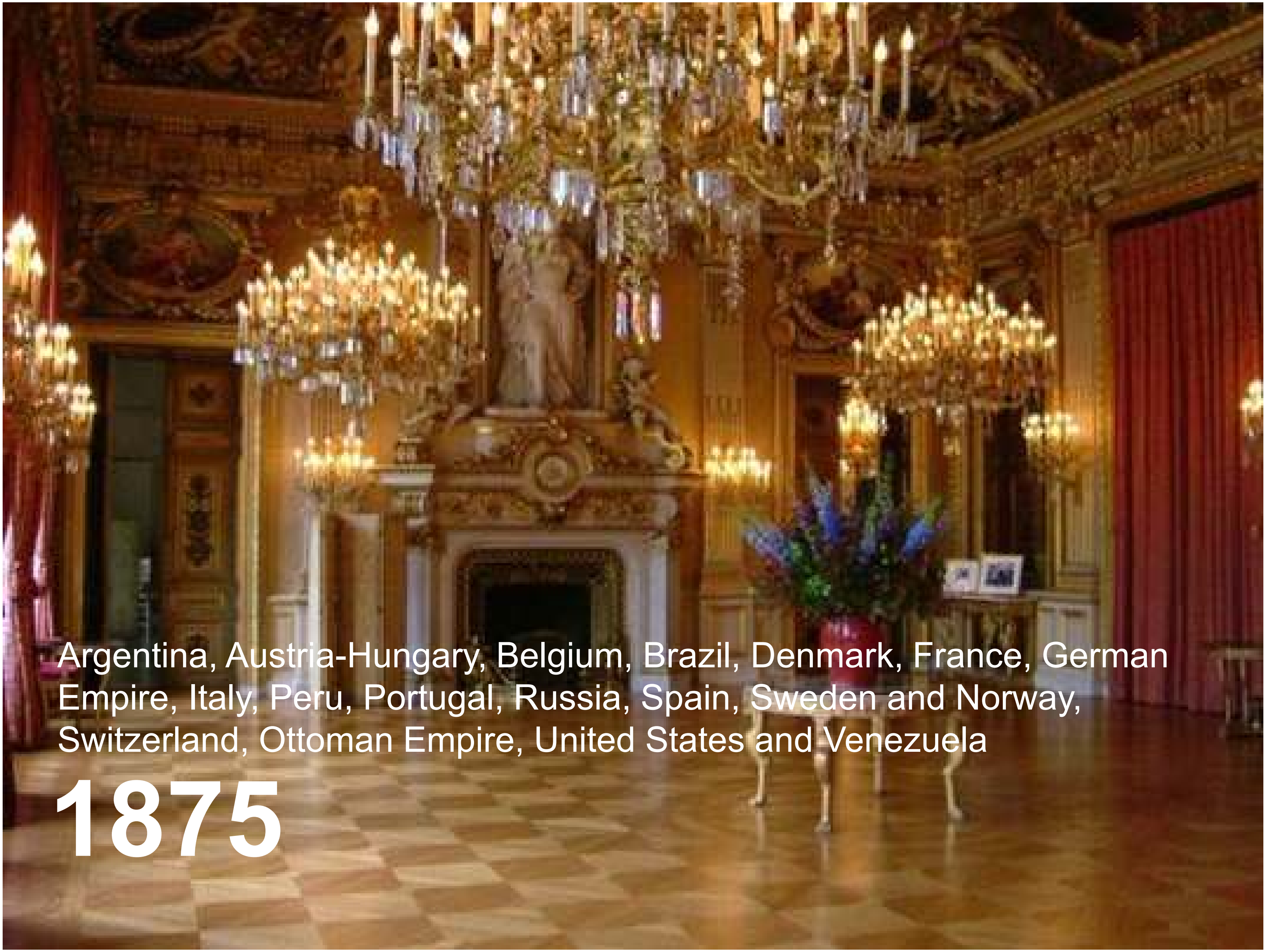
Canada

It is as easy to count atomies as to resolve the propositions of a lover..

As You Like It

William Shakespeare 1564-1616




Argentina, Austria-Hungary, Belgium, Brazil, Denmark, France, German Empire, Italy, Peru, Portugal, Russia, Spain, Sweden and Norway, Switzerland, Ottoman Empire, United States and Venezuela
1875

-May 20 1875, BIPM, CGPM and the CIPM was established, and a three-dimensional mechanical unit system was setup with the base units metre, kilogram, and second.

-1901 Giorgi showed that it is possible to combine the mechanical units of this metre–kilogram–second system with the practical electric units to form a single coherent four-dimensional system

-In 1921 Consultative Committee for Electricity (CCE, now CCEM)

-by the 7th CGPM in 1927. The CCE to proposed, in 1939, the adoption of a four-dimensional system based on the metre, kilogram, second, and ampere, the MKSA system, a proposal approved by the CIPM in 1946.

-In 1954, the 10th CGPM, the introduction of the ampere, the kelvin and the candela as base units

-in 1960, 11th CGPM gave the name International System of Units, with the abbreviation SI.

-in 1970, the 14th CGMP introduced mole as a unit of amount of substance to the SI


Le Système
international d'unités
The International
System
of Units
SI

1960

Dalton publishes first set of atomic weights and symbols in 1805

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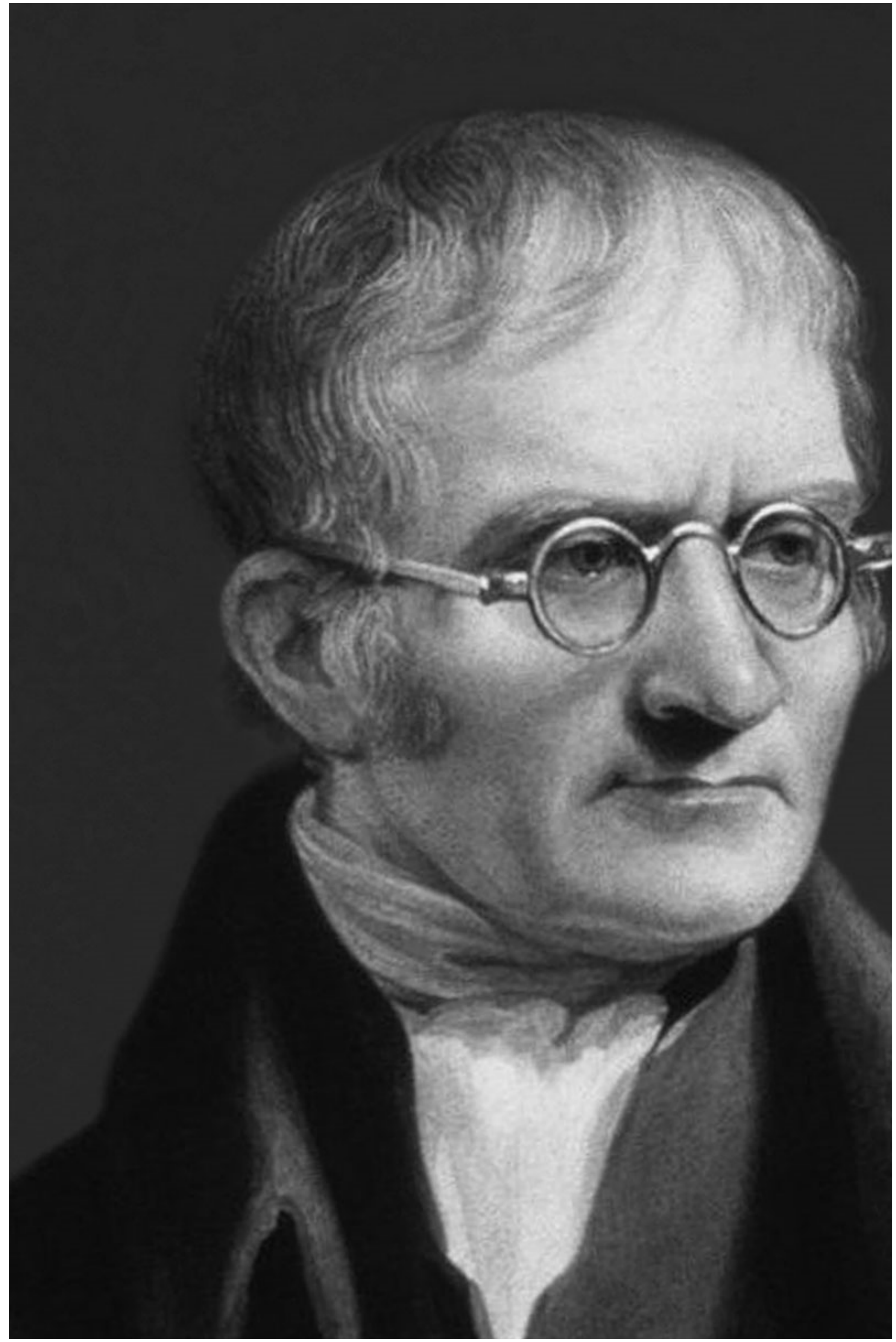
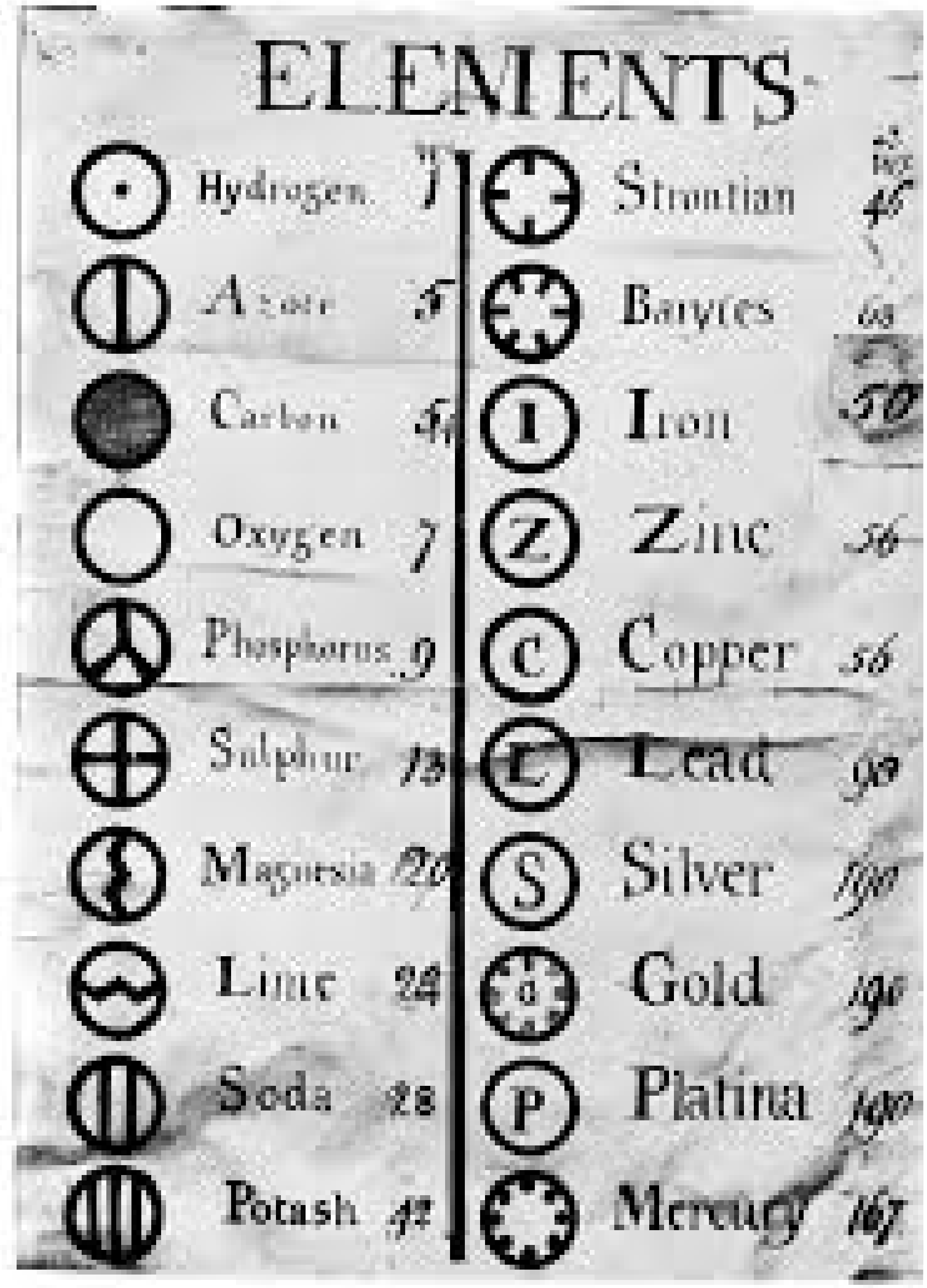


John Dalton(1766-1844)

Dalton publishes first set of atomic weights and symbols in 1805.



John Dalton(1766-1844)

Much improved atomic weight estimates, oxygen = 100

.

Jöns Jacob Berzelius (1779–1848)

Further improved atomic weight estimates

Stanislao Cannizzaro (1826–1910)

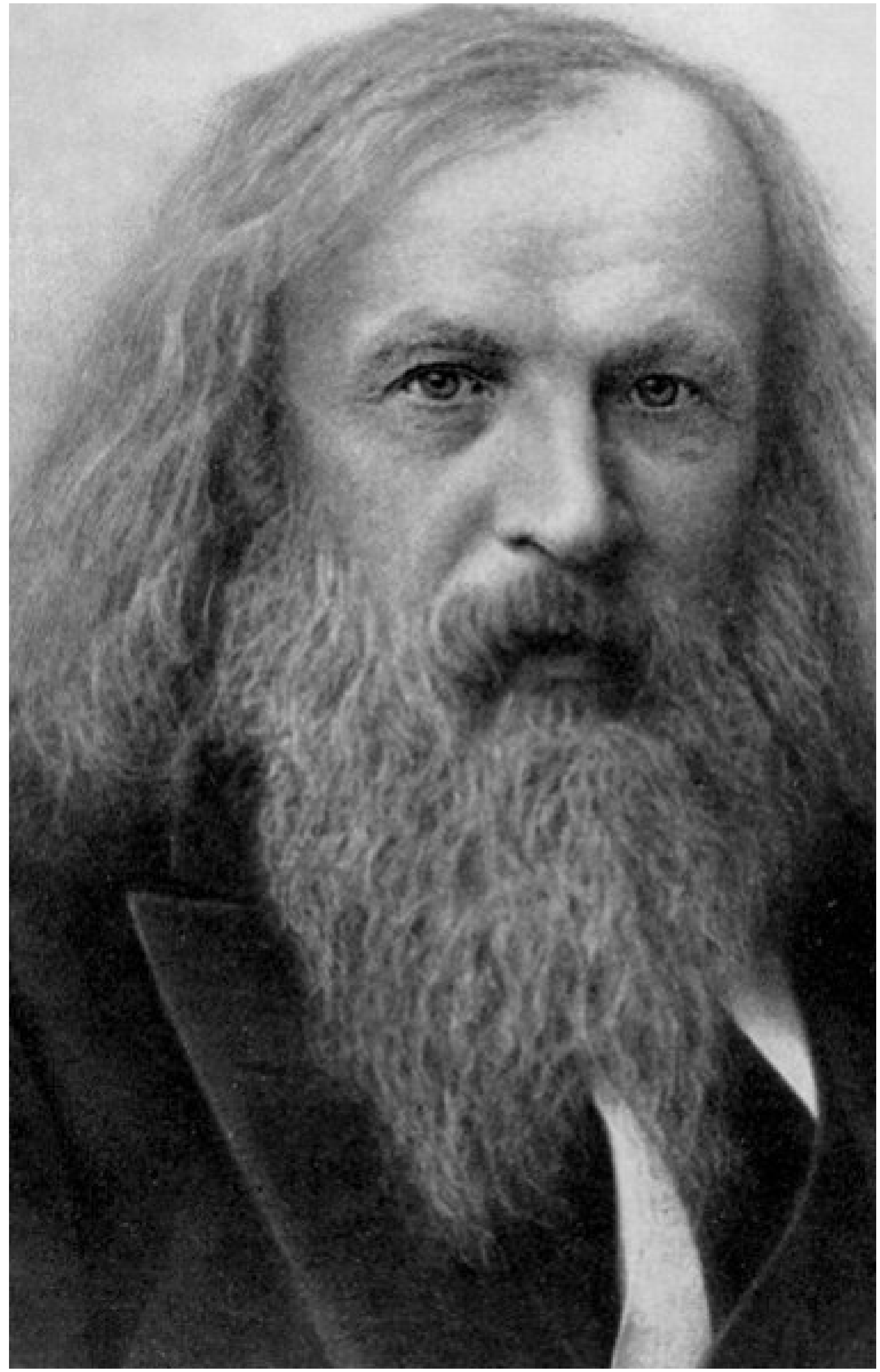
Karlsruhe Congress September 1860

"More precise definition of what is meant by the expressions: atom, molecule, equivalence, atomicity, basicity, and designated expressions; investigation as to the true equivalent of bodies and their formulas; introduction of a proportional description and a rational nomenclature…"

Birth of IUPAC

Carl Weltzien (1813–1870)

Periodic table, 1879



Dmitri Mendeleev (1834 –1907)

United Nations
Educational, Scientific and
Cultural Organization

International Year
of the Periodic Table
of Chemical Elements

First use of term “molar” in a sense of macroscopic mass *vis-à-vis* microscopic, “molecular” mass

A. W. Hofmann, *Introduction to Modern Chemistry, Experimental and Theoretic*, Walton and Maberley: London,
1865,

August Wilhelm Hofmann (1818-1892)

First use the mole as a noun in a sense that mass in grams directly reflects the mass of its constituent atoms molecules

W. Ostwald, Grundlagen der anorganischen Chemie, Engelmann: Leipzig, 1900.

Wilhelm Ostwald (1853-1932)

24th meeting of the General Conference on Weights and Measures

Paris, 17-21 October 2011

On the possible future revision of the International System of Units, the SI

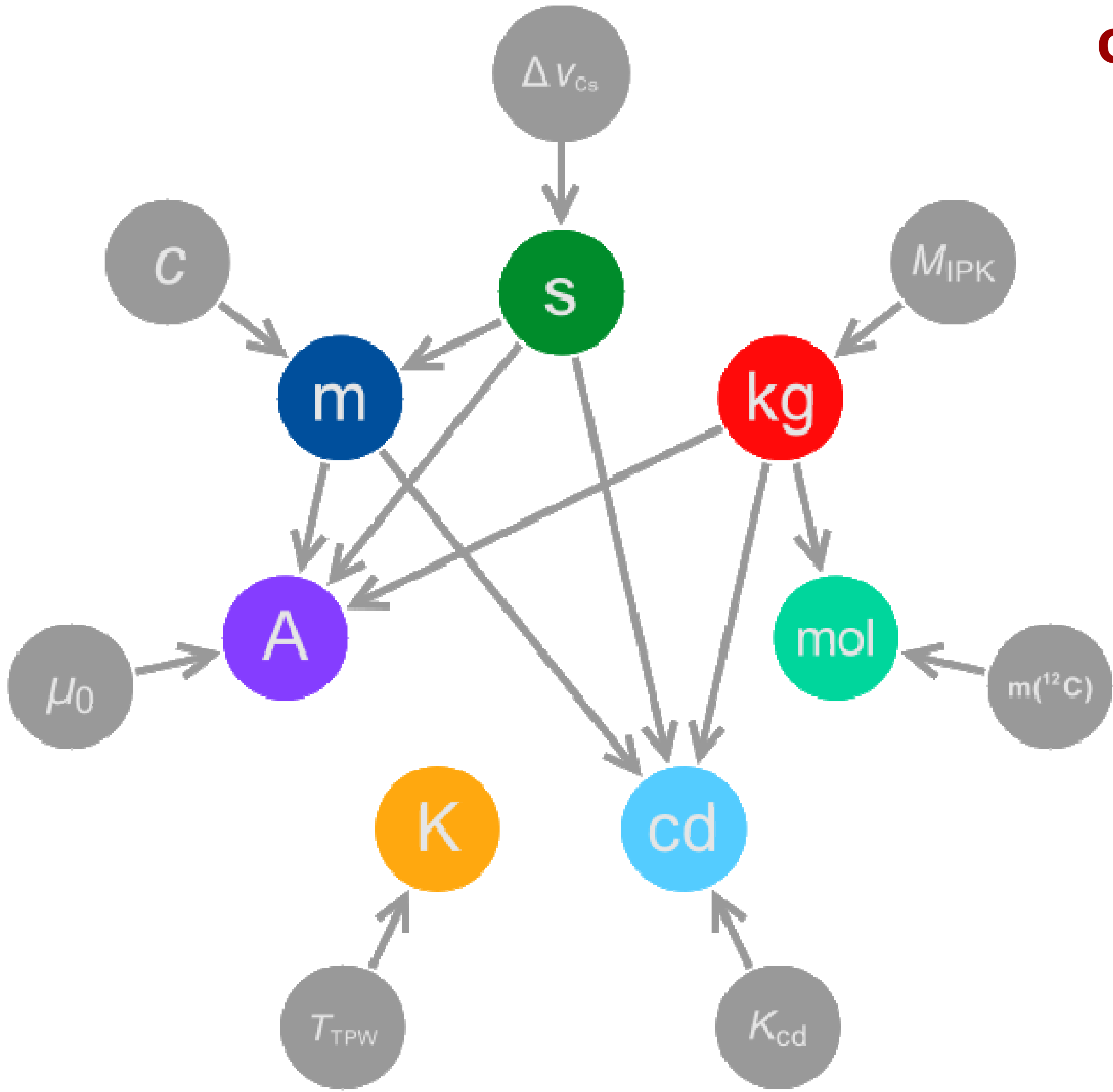
Resolution 1

takes note of the intention of the International Committee for Weights and Measures to propose a revision of the SI as follows:

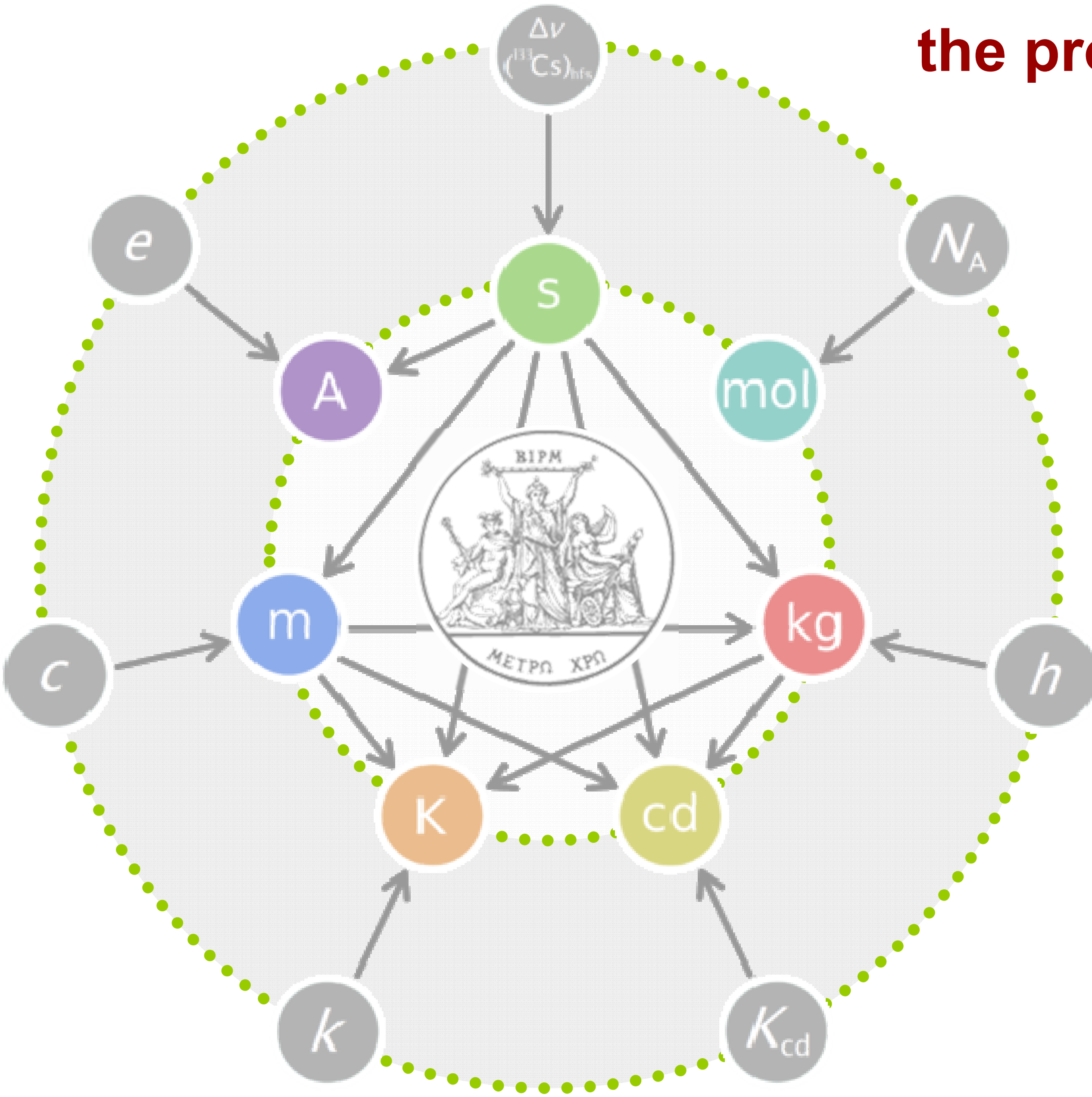
the International System of Units […] will be the system of units in which […] the Planck constant *h* is exactly 6.626 06X $\times 10^{-34}$ joule second, […]

2011

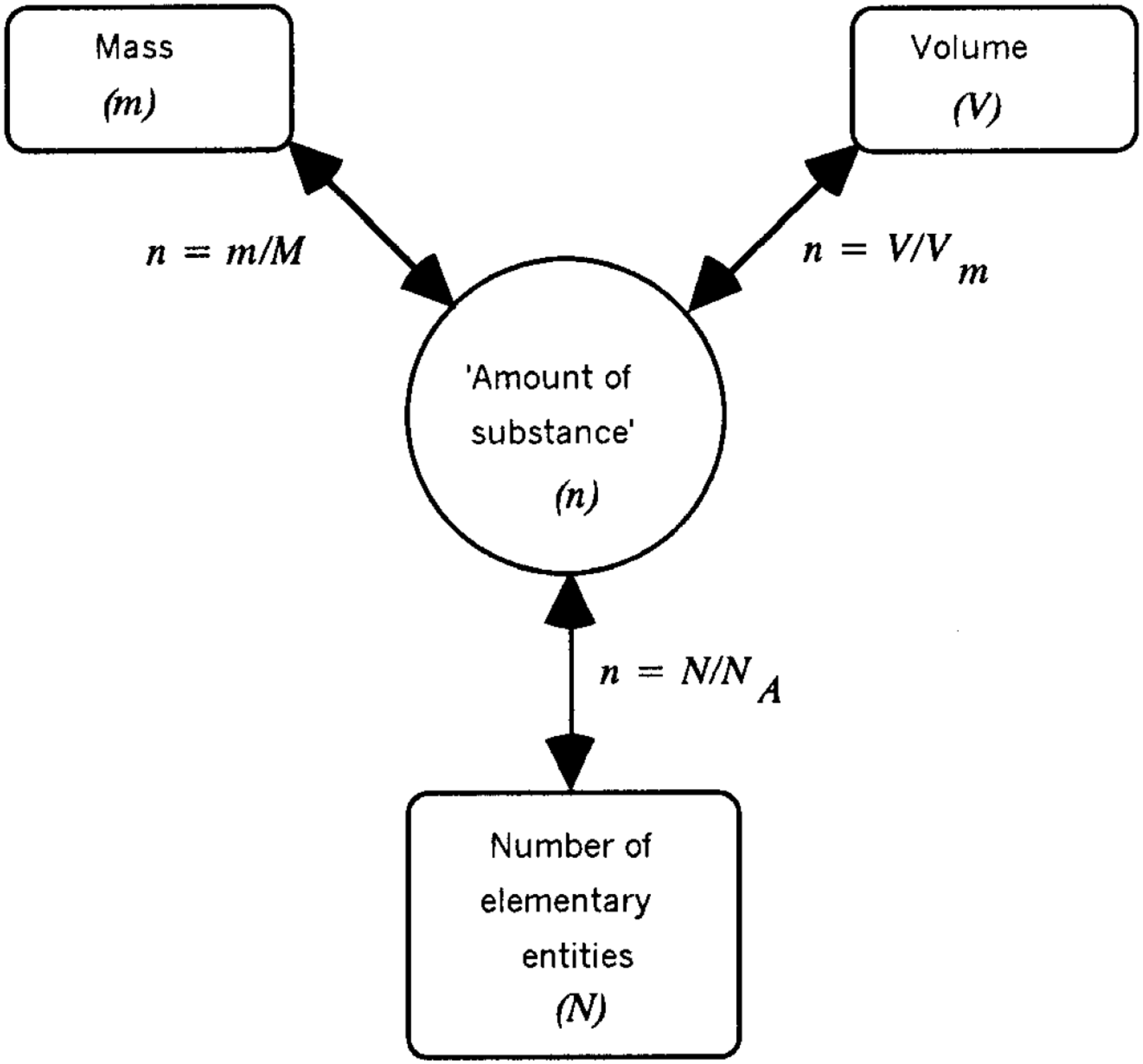
current SI



the proposed new-SI



The ‘amount of substance’ in relation to other quantities



The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram.

vs

The kilogram, kg, is the unit of mass; and it is defined by the Planck constant….

1. The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12; its symbol is 'mol'.

2. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

New wording is needed!!

Consultative Committee for Units (CCU)

President:	Prof. J. Ullrich President of the PTB, Vice-President of the CIPM Physikalisch-Technische Bundesanstalt Germany
Executive Secretary:	Dr E. de Mirandés CCU Executive Secretary Bureau International des Poids et Mesures France
Member(s):	• Centro Español de Metrología [CEM], Madrid • Commission internationale de l'éclairage [CIE] • Committee on Data for Science and Technology [CODATA Task Group on Fundamental Constants] • Federal Agency on Technical Regulating and Metrology [Rosstandart], Moscow • Federal Institute of Metrology METAS [METAS], Bern-Wabern • International Astronomical Union [IAU] • International Commission on Radiation Units and Measurements [ICRU] • International Electrotechnical Commission [IEC] • International Federation of Clinical Chemistry and Laboratory Medicine [IFCC], Milan • International Organization for Standardization [ISO] • International Organization of Legal Metrology [OIML], Paris • International Union of Pure and Applied Chemistry [IUPAC] • International Union of Pure and Applied Physics [IUPAP] • Korea Research Institute of Standards and Science [KRISS], Daejeon • Laboratoire National de Métrologie et d'Essais [LNE], Paris • National Institute of Metrology [NIM], Beijing • National Institute of Standards and Technology [NIST], Gaithersburg • National Metrology Institute of Japan, AIST [NMIJ/AIST], Tsukuba • National Physical Laboratory [NPL], Teddington • National Research Council of Canada [NRC], Ottawa • Physikalisch-Technische Bundesanstalt [PTB], Braunschweig
Personal member(s):	• Prof. M. Himbert • Dr T.J. Quinn
Honorary member(s):	• Prof. I.M. Mills, OBE FRS

CCU summary

- General information
- Members of the CCU
- CCU working groups
- CCU publications
- Photographs of the CCU
- Criteria for membership of the CCU

See also:

- CODATA Task Group on Fundamental Constants

Governance

- Criteria for membership of the CCU
- Rules of procedure for the CCs and their WGs

The mole, mol, is the unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles; **its magnitude is set by fixing the numerical value of the Avogadro constant to be equal to exactly 6.02214X×10^{23} when it is expressed in the unit mol^{-1}**.

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

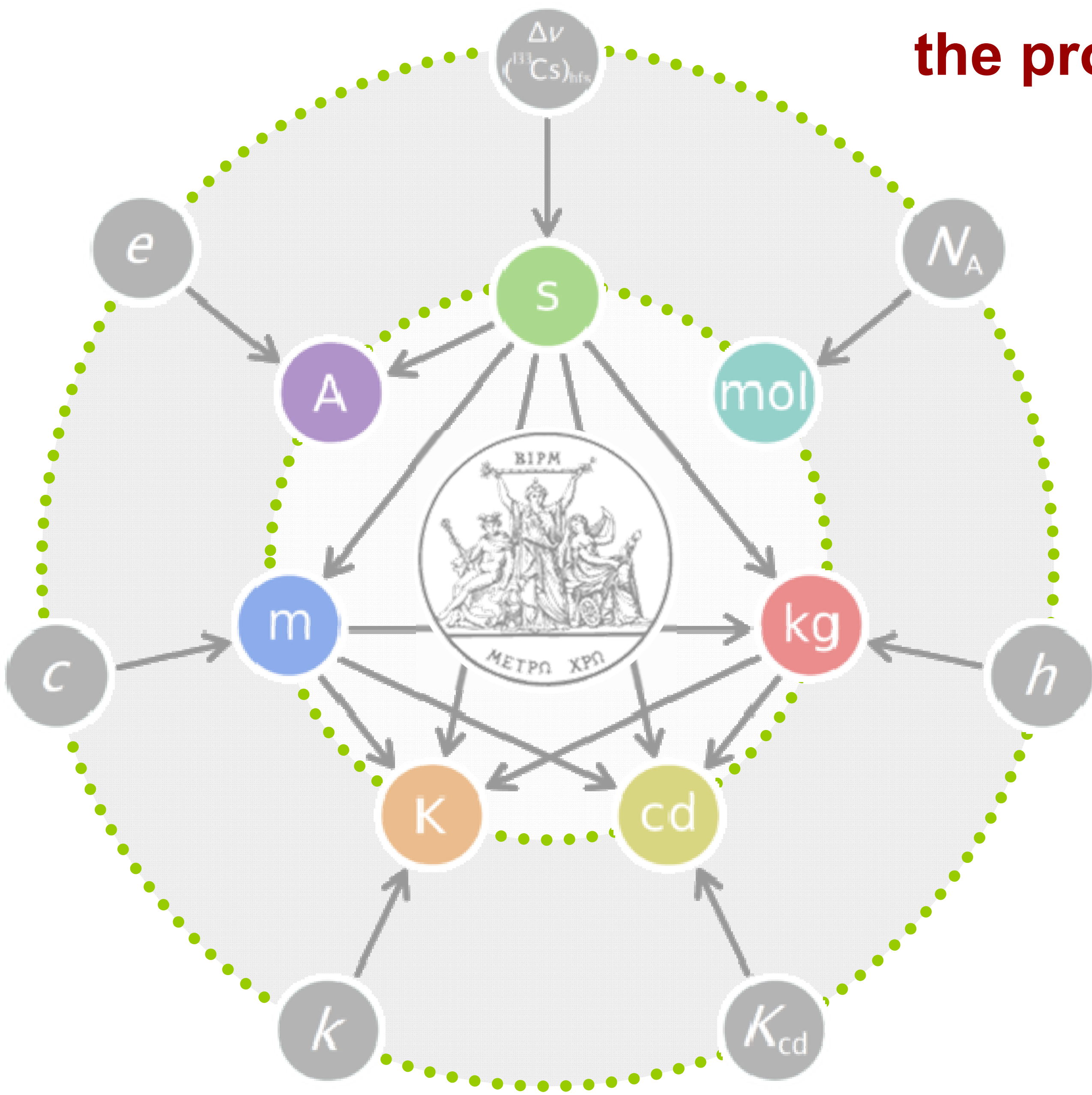
A CRITICAL REVIEW OF THE PROPOSED DEFINITIONS OF FUNDAMENTAL CHEMICAL QUANTITIES AND THEIR IMPACT ON CHEMICAL COMMUNITIES

Project team members:
Roberto Marquardt, Juris Meija, Zoltán Mester, Marcy Towns, Ron Weir, Richard Davis and Jürgen Stohner

The report

Roberto Marquardt, Juris Meija, Zoltán Mester, Marcy Towns, Ron Weir, Richard Davis and Jürgen Stohner, "A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities (IUPAC Technical Report)", *Pure Appl. Chem*. 89(7), pp. 951-981 (2017), https://doi.org/10.1515/pac-2016-0808

the proposed new-SI



The goal

kg	**< 20 μg**
h **or** N_A	**< 2 in** 10^8

the Avogadro constant and the Planck constant

If m_e is expressed in daltons, then

$$R_\infty = \frac{\alpha^2 m_e c}{2 N_A h}$$

CODATA **2010**	u_r
c	0
R_∞	5×10^{-12}
α	3×10^{-10}
m_e	4×10^{-10}

$$N_A \mapsto h$$

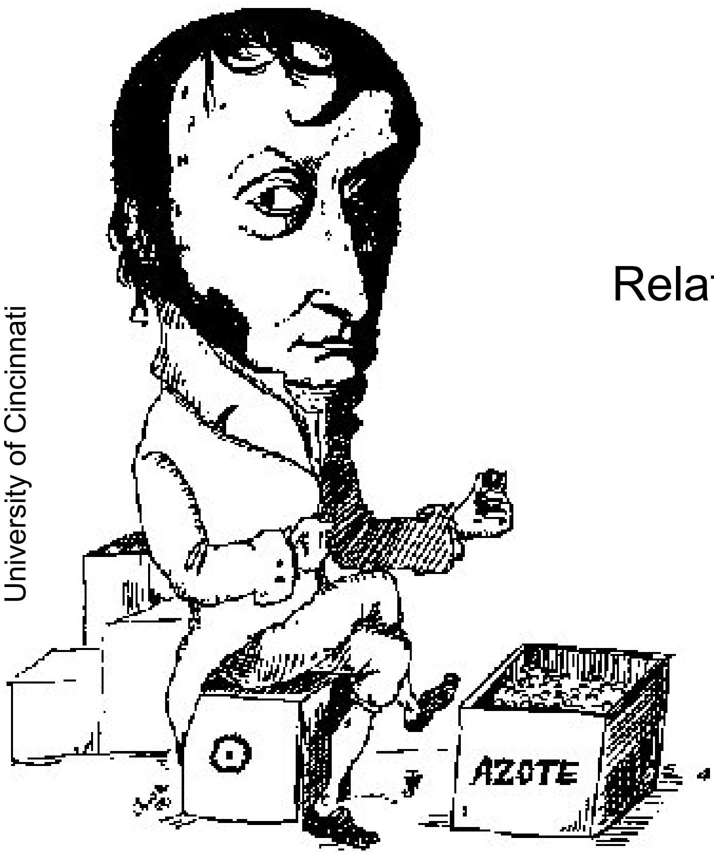
Planck constant: the Watt Balance

Planck constant: the Watt Balance

Compares a measurement of electrical and mechanical power.

the Avogadro constant

$$\boldsymbol{N}_{\mathbf{A}} = \frac{N(\mathrm{Si})}{m(\mathrm{Si})\,/A_{\mathrm{r}}(\mathrm{Si})}$$



SOURCE | Bill Jensen
University of Cincinnati

Relates the **kilogram** and the **atomic unit of mass**

Gläser and Borys *Rep Prog Phys* **2009** (72) 126101

The Avogadro constant

MEASUREMENT

Carl Sagan's method

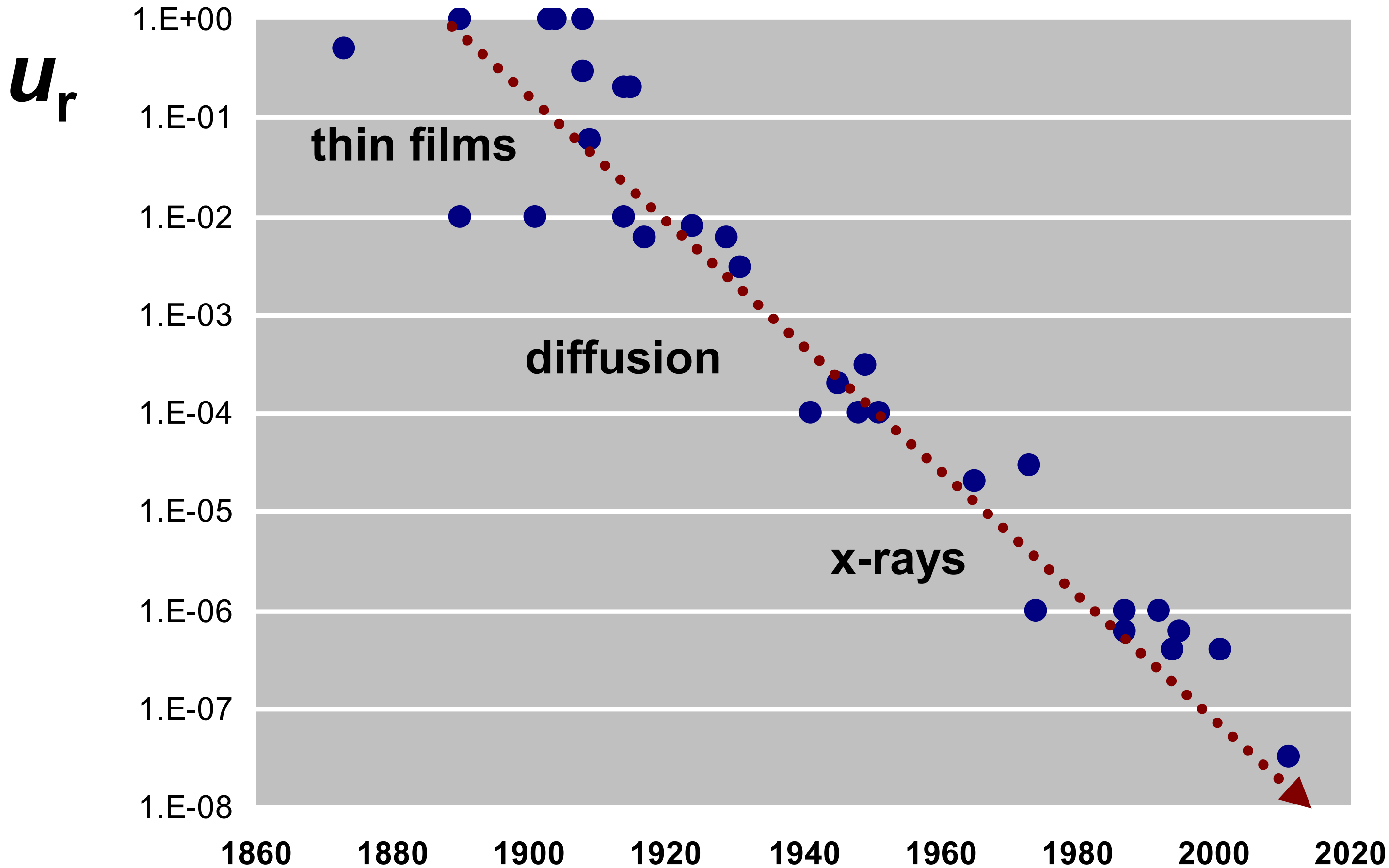
Put a known amount (volume and mass) of a hydrocarbon on a water and wait for the slick to diffuse to the maximum contiguous area.

Divide the original volume by that area and to get an estimate for the length of the molecule (*l*) and, thus, the volume it occupies (*l*^{3}).

$$N(x) = V / l^3$$

$$\boldsymbol{N}_\mathbf{A} = \frac{V / l^3}{m / m_a}$$

The Avogadro constant



Becker (2003) *Metrologia* 40: 366

Avogadro experiment

Avogadr   tween the
kilogram

A near-p   s density
is determ   ic level.

m   3]
m

The ratio   onstant.

Atomic weight measurements

Appendix C: The uncertainty budget

atomic weight	**61.7%**
lattice spacing	**30.4%**
radius	**6.0%**
…	

c.2000s

Becker (2003) *Metrologia* 40: 271-287

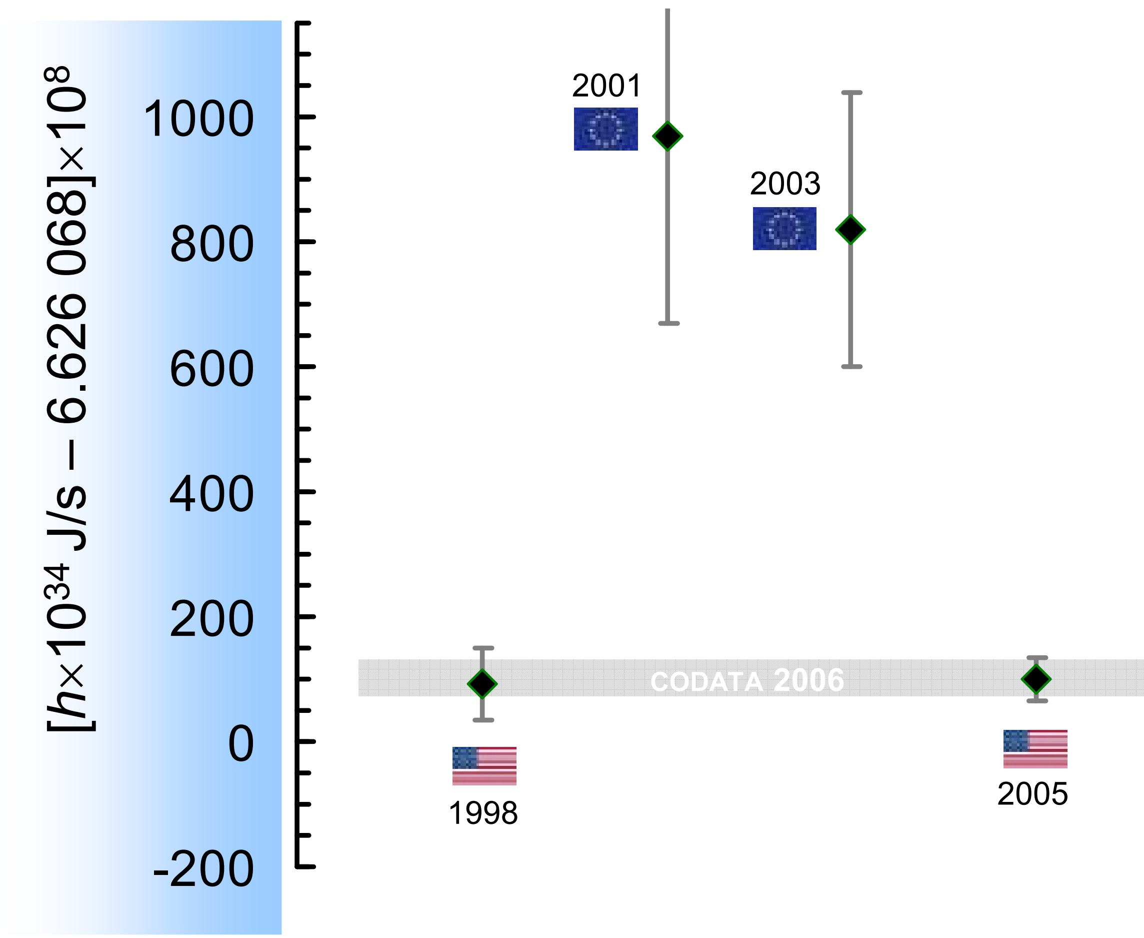
Atomic weight

$$A_r(\mathrm{Si})\, m_u = x_{28} m_{28} + x_{29} m_{29} + x_{30} m_{30}$$

Amount average mass of an element

E = hν

Planck constant 2005



Atomic weight

$$A_r(\mathrm{Si})\, m_u = x_{28} m_{28} + x_{29} m_{29} + x_{30} m_{30}$$

Amount average mass of an element

the Avogadro constant

Isotopic composition measurement demands

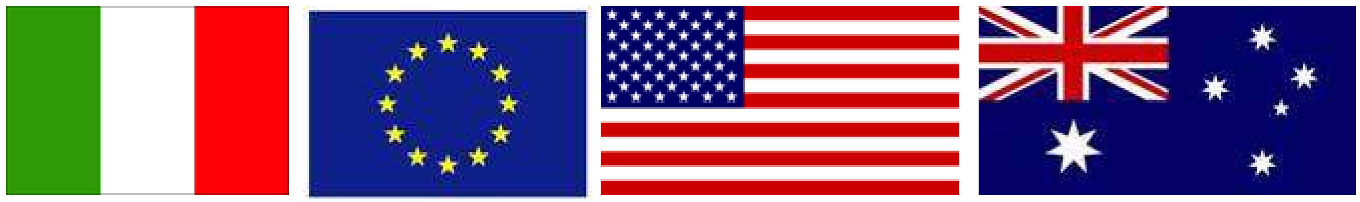
$u_r = 1 \times 10^{-8}$

$$N_A = \frac{N(\mathrm{Si})}{m(\mathrm{Si})/A_r(\mathrm{Si})}$$

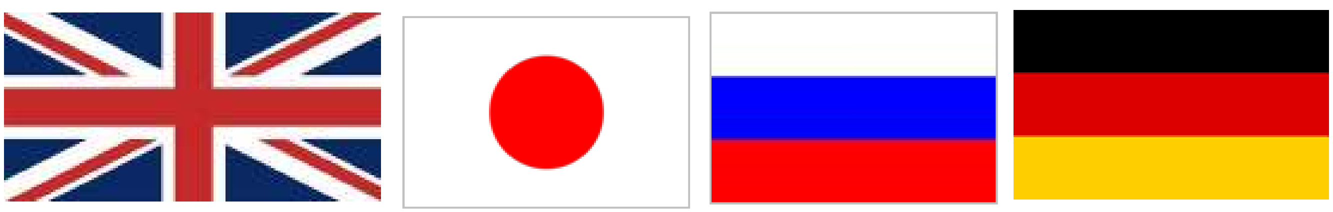
1994-2003	[1]	90% ^{28}Si	did result in $A_r(\mathrm{Si})$	$uA_r = 1 \times 10^{-6}$
2008-2011	[2]	99.99% ^{28}Si	could result in $A_r(\mathrm{Si})$	$uA_r = 1 \times 10^{-9}$
2012-?	[3]	99.99999% ^{28}Si	could result in $A_r(\mathrm{Si})$	$uA_r = 1 \times 10^{-12}$

$$m(\mathrm{Si}) \circ V(\mathrm{Si}) \circ d_{220} \circ A_r(\mathrm{Si})$$

the International Avogadro Coordination



$$m(\mathrm{Si}) \circ V(\mathrm{Si}) \circ d_{220} \circ A_r(\mathrm{Si})$$



Final report (Si): *IEEE Trans. Instr. Meas.* (2005) 54: 854-859

Final report (^{28}Si): *Phys. Rev. Lett.* (2011) 106, 030801

Manufacturing timeline of the 99.99% ^{28}Si monocrystal

$SiF_4 \rightarrow {}^{28}SiF_4$

Centrifugal isotope enrichment

Centrotech
St Petersburg (Russia)

$^{28}SiF_4 \rightarrow {}^{28}SiH_4 \rightarrow {}^{28}Si$ (poly)

Chemical purification
Chemical vapor deposition

Institute of Chemistry of High-Purity Substances
Russian Academy of Sciences
Nizhny Novgorod (Russia)

^{28}Si (poly) $\rightarrow {}^{28}Si$ (mono)

Growth of the monocrystal

Leibniz Institute for Crystal Growth
Berlin (Germany)

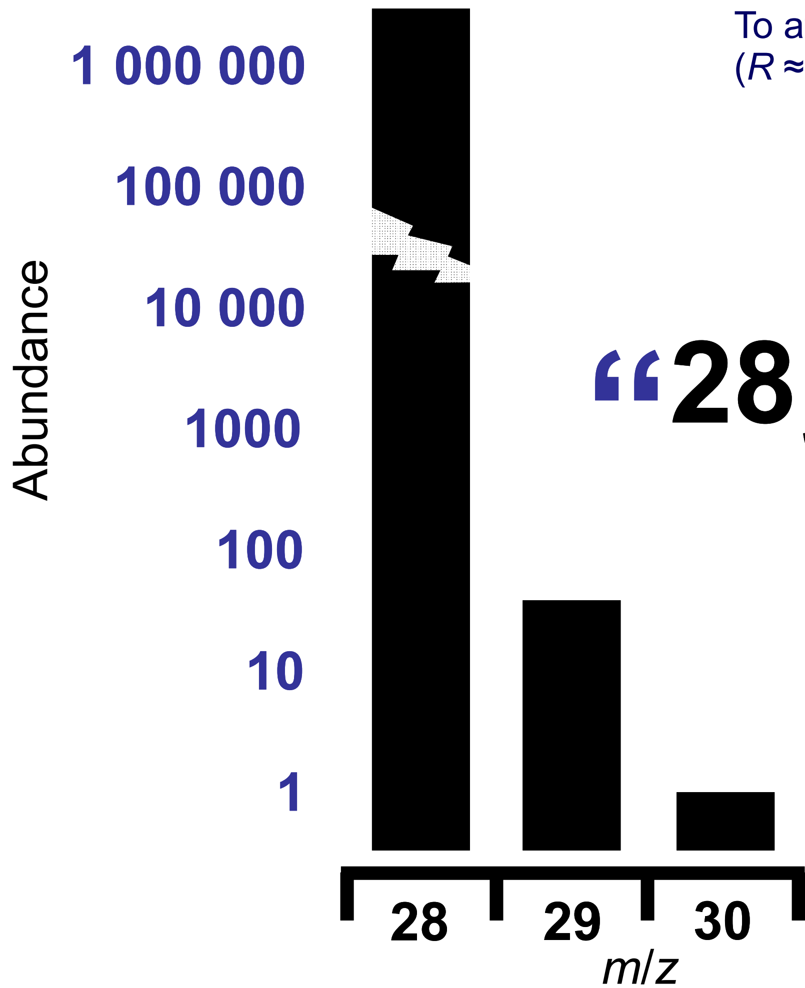
Manufacturing completed in 2007 and
the 5 kg monocrystal is available for analysis since 2008.

Multicollector-ICP-MS **vs** **Isotope ratio MS**

SOURCE | Thermo Scientific

Atomic weight determination: *direct approach*

To attain 10^{-8} relative uncertainty, the $^{28}Si/^{29}Si$ ratio ($R \approx 25\ 000:1$) has to be measured to within 1%.



“^{28}Si”

^{28}Si	1000 V
^{29}Si	50 mV
^{30}Si	1 mV

International Journal of Mass Spectrometry
Volume 289, Issue 1, 1 January 2010, Pages 47-53

Novel concept for the mass spectrometric determination of absolute isotopic abundances with improved measurement uncertainty: Part 1 – theoretical derivation and feasibility study

Olaf Rienitz, Axel Pramann, Detlef Schiel

Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany

Received 3 September 2009, Revised 22 September 2009, Accepted 23 September 2009, Available online 30 September 2009.

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https://doi.org/10.1016/j.ijms.2009.09.010 Get rights and content

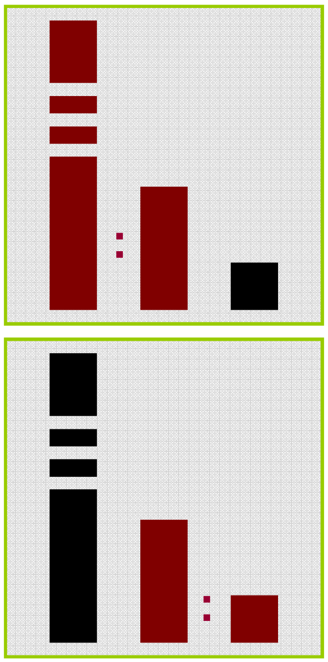
Abstract

The development of a new method for the experimental determination of absolute isotopic abundances using a modified isotope dilution mass spectrometry (IDMS) technique is described. The intention and thus main application will be the quantification of molar masses *M* of highly enriched materials with improved

Atomic weight determination

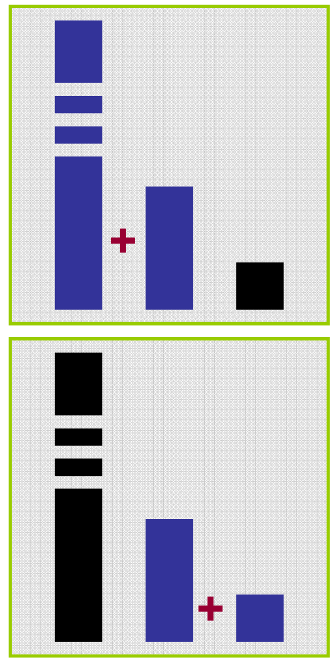
variable transformation

$R_{28/29} \bullet R_{30/29}$



$$\bar{m}_{Si} = \frac{\sum m_i R_i}{\sum R_i}$$

$w_{28+29} \bullet w_{29+30}$



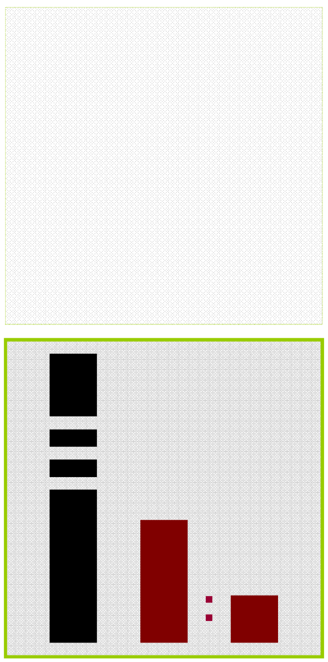
$$\bar{m}_{Si} = \frac{\sum w_i}{\sum w_i / m_i}$$

Based on AB (   ) and AC (   )

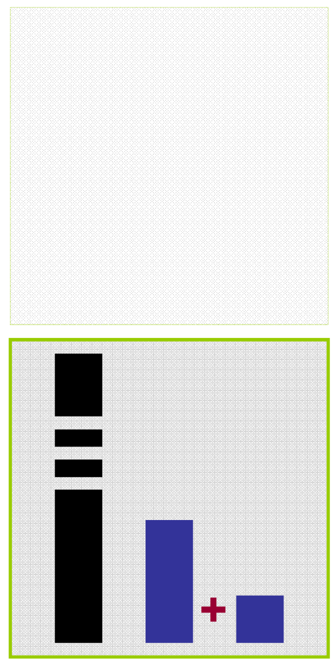
Atomic weight determination

variable transformation

$R_{28/29}$ • $R_{30/29}$



w_{28+29} • w_{29+30}



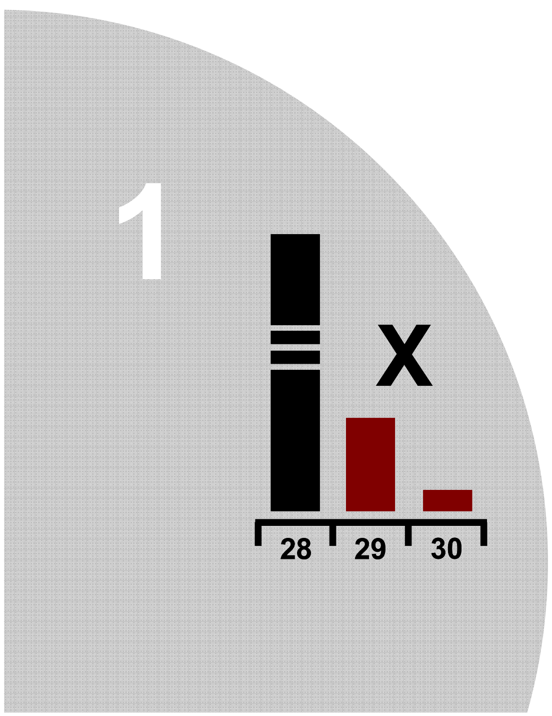
$$A_r(\mathrm{Si})\, m_u = \frac{m_{28}\sum m_i R_i}{m_{28}(1-w_{28})\sum R_i + w_{28}\sum m_i R_i}$$

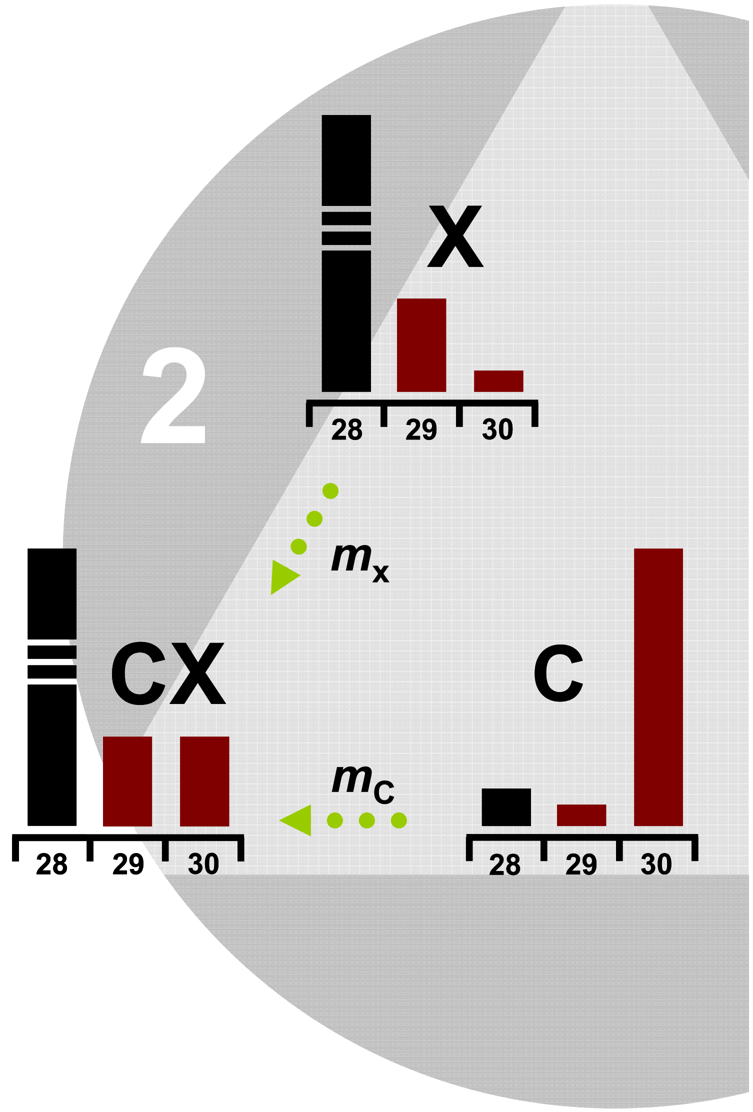
Based on AB ( ) and AC ( )

Atomic weight determination in silicon-28

$R_{28/29}$ • $R_{30/29}$

w_{28+29} • w_{29+30}





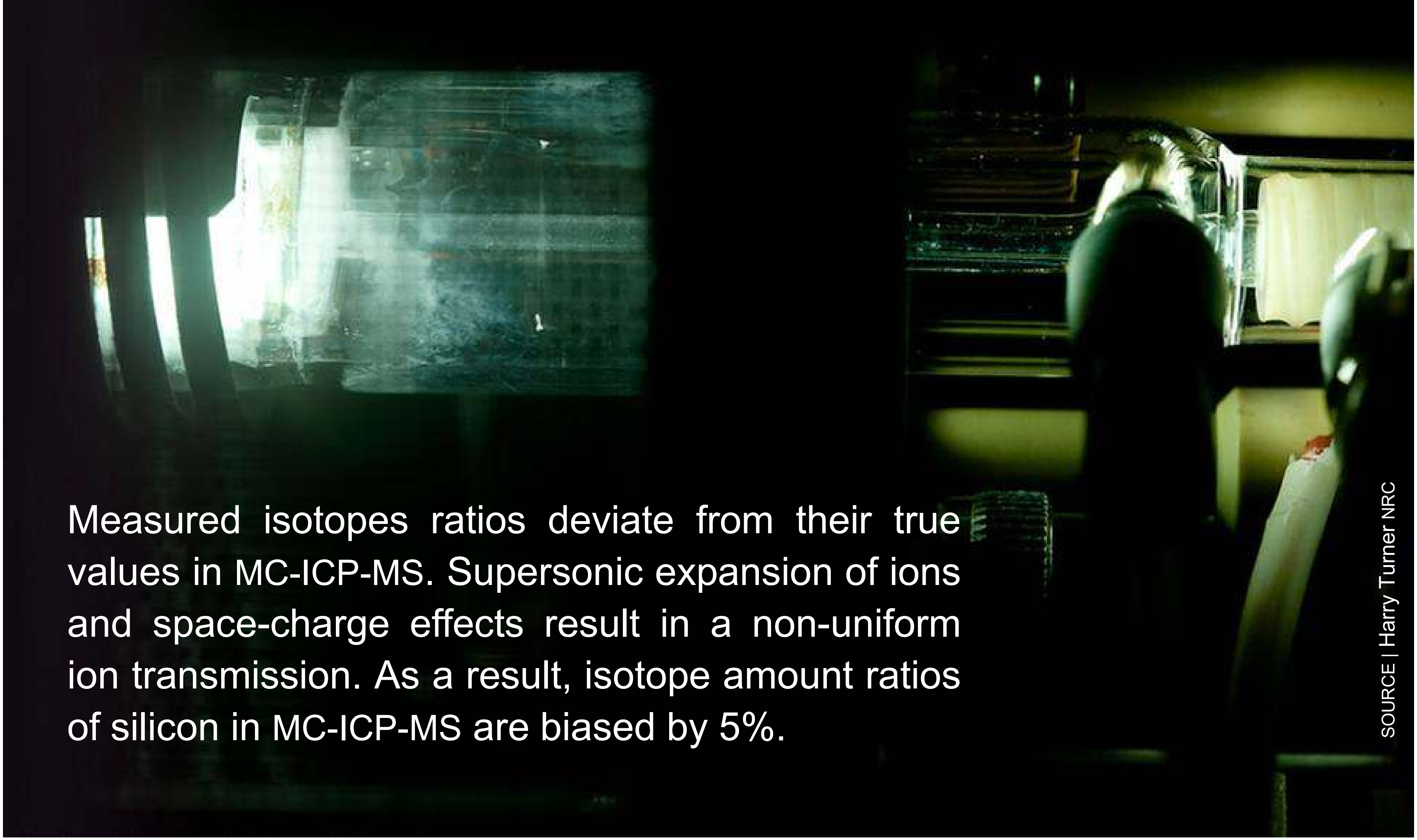
Uncertainty analysis of the atomic weight

Using the measurement strategy as outlined above, only two variables contribute significantly to the atomic weight uncertainty of the near-pure ^{28}Si:

$$u_r = 1 \times 10^{-8}$$

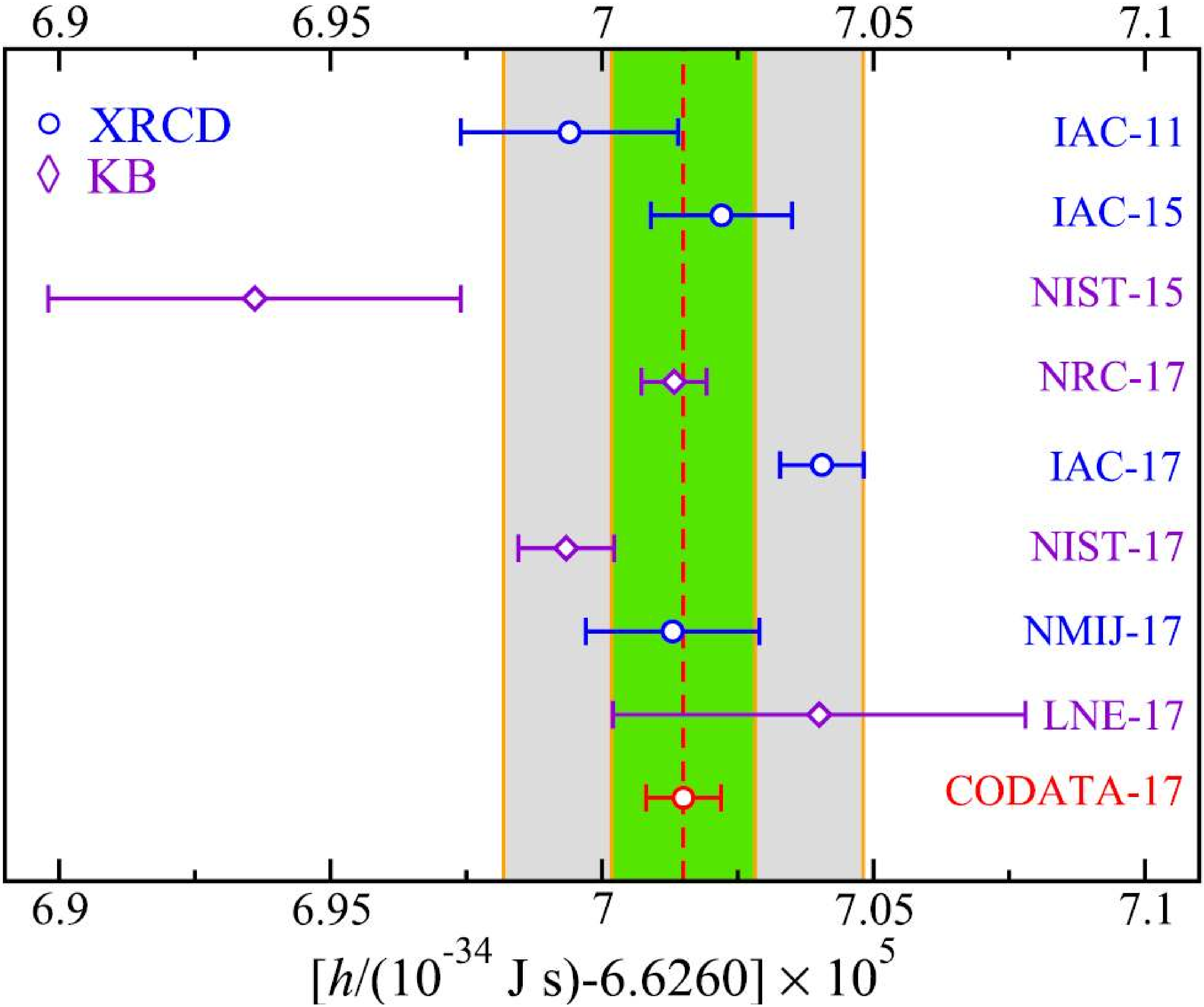
$R_{30/29}$ in the material **X**	u_r = 10% … 5%
$R_{30/29}$ in the blend **CX**	u_r = 0.5% … 1%

2. Calibration of isotope amount ratios



Measured isotopes ratios deviate from their true values in MC-ICP-MS. Supersonic expansion of ions and space-charge effects result in a non-uniform ion transmission. As a result, isotope amount ratios of silicon in MC-ICP-MS are biased by 5%.

SOURCE | Harry Turner NRC



6.9
6.95
7
7.05
7.1
XRCD
KB
IAC-11
IAC-15
NIST-15
NRC-17
IAC-17
NIST-17
NMIJ-17
LNE-17
CODATA-17
$[h/(10^{-34}\ \mathrm{J\ s})-6.6260]\times 10^{5}$

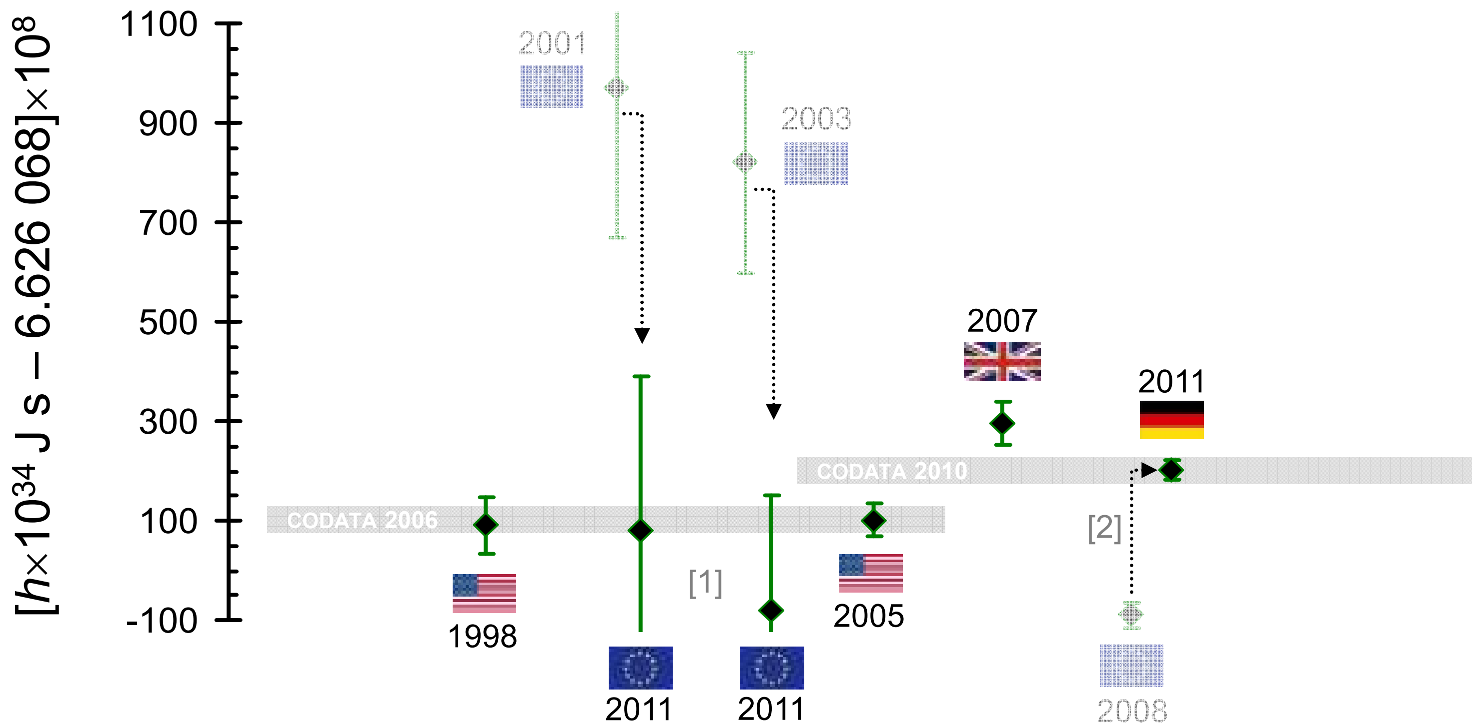
The CODATA 2017 values of h, e, k, and N_A for the revision of the SI

Quantity	Value	Rel. stand. uncert u_r
h	$6.626\,070\,150(69) \times 10^{-34}$ J s	1.0×10^{-8}
e	$1.602\,176\,6341(83) \times 10^{-19}$ C	5.2×10^{-9}
k	$1.380\,649\,03(51) \times 10^{-23}$ J K^{-1}	3.7×10^{-7}
N_A	$6.022\,140\,758(62) \times 10^{23}$ mol^{-1}	1.0×10^{-8}

D B Newell *et al* 2018 *Metrologia* **55** L13

Planck constant, *h*

[1] Valkiers et al. *Metrologia* **2011** (48) S26-S31
[2] Pramann et al. *Metrologia* **2011** (48) S20-S25



Impact of the redefinition on chemical metrology

Characterization of impurities in high purity materials

Isotope ratio measurements

Decision	Date
Decision CIPM/107-7	June 2018
The CIPM noted the steps taken to implement its decisions regarding the future of the BIPM Pension Fund and re-iterated its commitment to achieve its long-term financial stability. *[Decisions]*	
Decision CIPM/107-8	June 2018
The CIPM requested the BIPM Director to commission an independent report presenting a range of options for the BIPM staff and operations, in the case that the planned measures to achieve long-term financial stability cannot be implemented in an effective and timely manner. *[Decisions]*	
Decision CIPM/107-9	June 2018
The CIPM decided to review the purpose and agenda of the meeting of the CC Presidents at the next meeting of the CIPM. *[Decisions]*	
Decision CIPM/107-10	June 2018
The CIPM approved the proposal of the CCQM to establish a CCQM Working Group on Isotope Ratio Measurement. *[Decisions]*	
Decision CIPM/107-11	June 2018
The CIPM asked the BIPM Director and Legal Advisor to explore options to formalize the BIPM liaison with the CODATA Task Group on Fundamental Constants. *[Decisions]*	
Decision CIPM/107-12	June 2018
It was brought to the attention of the CIPM that there is a discrepancy relating to the definition of the term "unit" between the draft 9th edition of the SI Brochure and the 8th edition. The CIPM asked the CCU President to organize a vote by correspondence among the CCU members, with a deadline of the end of August 2018, as to whether to retain the wording of the draft 9th edition or to revert to the wording of the 8th edition, and to report back to the CIPM President for further action (if necessary). *[Decisions]*	
Decision CIPM/107-13	June 2018
The CIPM agreed with the proposal from the CCU President to establish a Task Group to review	

The goal has been reached

kg $< 20\ \mu g$

h* or *N_A < 2 in 10^8

New definition of mole

Roberto Marquardt, Juris Meija, Zoltán Mester, Marcy Towns, Ron Weir, Richard Davis and Jürgen Stohner, "Definition of the mole (IUPAC Recommendation 2017)", *Pure Appl. Chem*. 90(1), pp. 175-180 (2018), https://doi.org/10.1515/pac-2017-0106

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New definition of mole

The mole, symbol mol, is the SI unit of amount of substance. **One mole contains exactly 6.022 140 76×10^{23} elementary entities.** This number is the fixed numerical value of the Avogadro constant, N_A, when expressed in mol^{-1}, and is called the Avogadro number.

The amount of substance, symbol *n*, of a system is a measure of the number of specified elementary entities. An elementary entity may be an atom, a molecule, an ion, an electron, any other particle or specified group of particles.

~~The mole is the amount of substance of a system that contains as many elementary entities as there are atoms in 0.012 kilogram of carbon-12.~~

New definition of mole

El mol, simbolo mol, es la unidad del SI de cantidad de sustancia. **Un mol contiene exactamente 6.022 140 76 x 10^{23} entidades elementales.** Este numero es el valor numerico fijo de la constante de Avogadro, N_A, cuando se expresa en mol^{-1}, y se llama numero de Avogadro.

~~El mol es la cantidad de sustancia de un sistema que contiene tantas entidades elementales como átomos hay en 0,012 kilogramos de carbono 12; su símbolo es “mol”.~~

IUPAC INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

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Questions, comments?

zoltan.mester@nrc.ca