SIM
SISTEMA INTERAMERICANO DE METROLOGÍA

SIM METROLOGY SCHOOL

A brief overview of the chemical metrology

SPEAKER

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Outline

- **Chapter 1.** Historical evolution of the mole
- **Chapter 2.** Basic Measurement principles in Chemistry
- **Chapter 3.** Structure of the CCQM and main focus areas
- **Chapter 4.** SIM WG-8 perspective
- **Chapter 5.** Current technical challenges and future trends

Clapeyron, Emile. (1834). “Memoir on the Motive Power of Heat.” Journal de l’Ecole Polytechnique, XIV, 153.

Chapter 1: Historical evolution of the mole

The mole: a brief history

Benoît Paul Émile Clapeyron (1834) work consolidated earlier observations made by Boyle, Charles, and Gay-Lussac into the equation of state "ideal gas law".

Émile Clapeyron (1853-1932)

$$PV = nRT$$

equation of state (ideal gas law)

Where:

- P is the pressure of the gas,
- V is the volume of the gas,
- n is the amount of substance of the gas (in moles),
- R is the ideal gas constant,
- T is the absolute temperature of the gas.

However, Clapeyron's original formulation of the ideal gas law was more conceptual and less about presenting the exact formula $PV = nRT$ as we know it today! So, mol definition at this time were more implicit than explicit!

Clapeyron, Emile. (1834). "Memoir on the Motive Power of Heat." Journal de l'Ecole Polytechnique, XIV, 153.

The mole: a brief history

Therefore, It was formally Wilhelm Ostwald (1853-1932) how introduced the “Mol” (mole in German), probably in 1893. However, he used this term to mean “molecular weight in gram”

Wilhelm Ostwald
(1853-1932)

$$PV = RT$$

(1893) $$mPV = GRT$$

$$PV = \frac{G}{m} RT$$

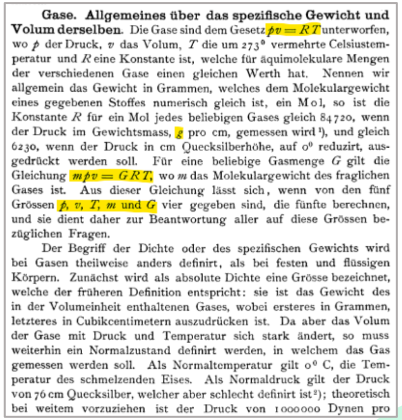
$$PV = nRT$$

equation of state
(ideal gas law)

“We generally call one mole the weight in grams (**G**) that is numerically identical with the molecular weight of a given substance (**m**)”

“mol practical determination”

$$n(x) = \frac{m(x)\ [g]}{M(x)\ [g/mol]}$$



Gase. Allgemeines über das spezifische Gewicht und Volum derselben. Die Gase sind dem Gesetz $pv = RT$ unterworfen, wo p der Druck, v das Volum, T die um 273° vermehrte Celsiustemperatur und R eine Konstante ist, welche für äquimolekulare Mengen der verschiedenen Gase einen gleichen Werth hat. Nennen wir allgemein das Gewicht in Grammen, welches dem Molekulargewicht eines gegebenen Stoffes numerisch gleich ist, ein Mol, so ist die Konstante R für ein Mol jedes beliebigen Gases gleich 84720, wenn der Druck im Gewichtsmass, g pro cm, gemessen wird [1]), und gleich 6230, wenn der Druck in cm Quecksilberhöhe, auf 0° reduzirt, ausgedrückt werden soll. Für eine beliebige Gasmenge G gilt die Gleichung $mpv = GRT$, wo m das Molekulargewicht des fraglichen Gases ist. Aus dieser Gleichung lässt sich, wenn von den fünf Grössen p, v, T, m und G vier gegeben sind, die fünfte berechnen, und sie dient daher zur Beantwortung aller auf diese Grössen bezüglichen Fragen.

Der Begriff der Dichte oder des spezifischen Gewichts wird bei Gasen theilweise anders definirt, als bei festen und flüssigen Körpern. Zunächst wird als absolute Dichte eine Grösse bezeichnet, welche der früheren Definition entspricht: sie ist das Gewicht des in der Volumeinheit enthaltenen Gases, wobei ersteres in Grammen, letzteres in Cubikcentimetern auszudrücken ist. Da aber das Volum der Gase mit Druck und Temperatur sich stark ändert, so muss weiterhin ein Normalzustand definirt werden, in welchem das Gas gemessen werden soll. Als Normaltemperatur gilt 0° C, die Temperatur des schmelzenden Eises. Als Normaldruck gilt der Druck von 76 cm Quecksilber, welcher aber schlecht definirt ist [2]); theoretisch bei weitem vorzuziehen ist der Druck von 1000000 Dynen pro

W. Ostwald. . , Leipzig, 1893. pp 119.

Marquardt, R. (2019). The mole and IUPAC: a brief history. Chemistry International, 41(3), 50-52.

The mole: a brief history

From 1900 to 2014, great advances were made in the definition of both: mole and Avogadro's number.

Change of the numerical value of the quantity which is presently known to be the Avogadro constant over time.

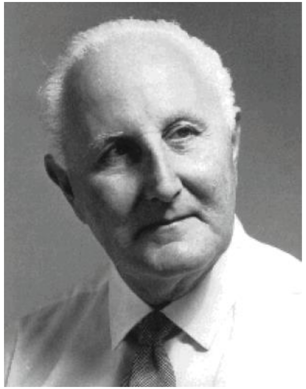
Name	Year	Numerical value	Notes
J.C. Magnenus	~1646	$\approx 2\times10^{22}$ [a]	Diffusion of incense
			Burnt in a church
Loschmidt	~1865	5.8×10^{23} [a]	Mean free path in gases
Röntgen, Rayleigh	~1890	$(6–7)\times10^{23}$	
Ostwald	~1899	6.3×10^{23} [a]	
Planck	1900	6.175×10^{23}	Black-body radiation
Einstein,	1905/6	6.17×10^{23}	
Smoluchowski	1908	6.0×10^{23}	
	1911	6.56×10^{23}	
Perrin	1909	6.5×10^{23}	
Rutherford	1909	6.16×10^{23}	Counting α-particles
Millikan	1917	6.064×10^{23}	Faraday's law
DuNouy	~1924	6.003×10^{23}	
Kappler	1931	6.059×10^{23}	
Birge	1941	6.02338×10^{23}	Crystal lattice/XRCD[b]
De Bièvre	2001	6.0221339×10^{23}	
Andreas *et al.*	2011	$6.02214078(18)\times10^{23}$	Crystal lattice/XRCD[b]
CODATA	2014	$6.022140857(74)\times10^{23}$	Recommended

[a]Recalculated, numbers originally given in terms of molecules per cm^3 or per piece of incense. [b]XRCD: X-ray crystal

Marquardt, R., Meija, J., Mester, Z., Towns, M., Weir, R., Davis, R., & Stohner, J. (2017). A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities (IUPAC Technical Report). Pure and Applied Chemistry, 89(7), 951-981.

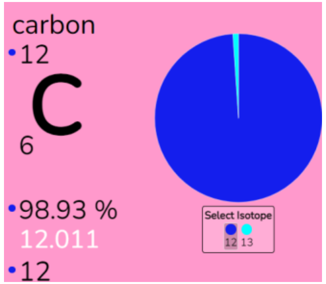
The mole: a brief history

However, it was Edward Guggenheim in 1961 how wrote:



Edward Guggenheim (1901–1970)

"The mole is the amount of substance containing the same number of molecules (or atoms or radicals or ions or electrons as the case may be) as there are atoms in 12 grams of ^{12}C."



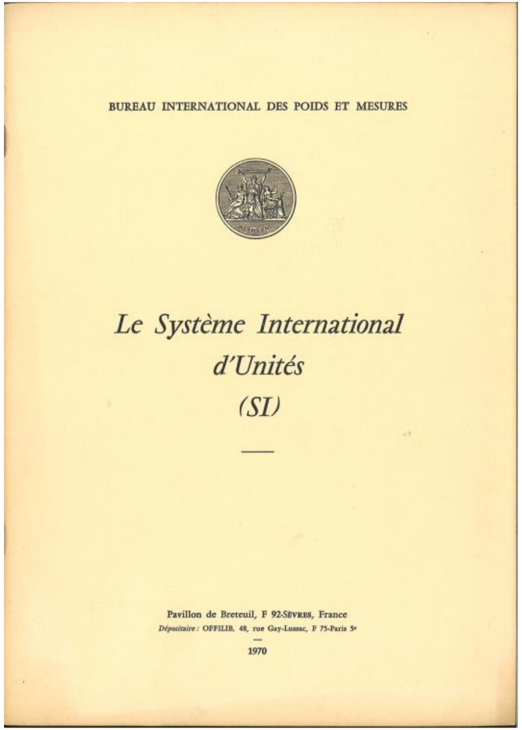
- ✓ Hight stability (unalterable)
- ✓ 98.93% Natural Abundance
- ✓ Molar mass: 12 g mol^{-1}
- ✓ Other isotopes are more complex (^{16}O, ^{17}O and ^{18}O)

Guggenheim was a member of the IUPAP and IUPAC. Moreover, both International Bodies have representation in the TC 12 (Quantities and units) of the ISO.

Guggenheim, E. A. (1961). The mole and related quantities. Journal of Chemical Education, 38(2), 86.

The mole: a brief history

In 1970 during the 14th General Conference of Weight and Measures (CGPM) the amount of substance (mole) were introduce as a new unit of the S.I:



Resolution 3:

SI unit of amount of substance (mole)

The 14th Conférence Générale des Poids et Mesures (CGPM),

considering the advice of the International Union of Pure and Applied Physics, of the International Union of Pure and Applied Chemistry, and of the International Organization for Standardization, concerning the need to define a unit of amount of substance,

decides

Strong relationship with kg!!

01 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".

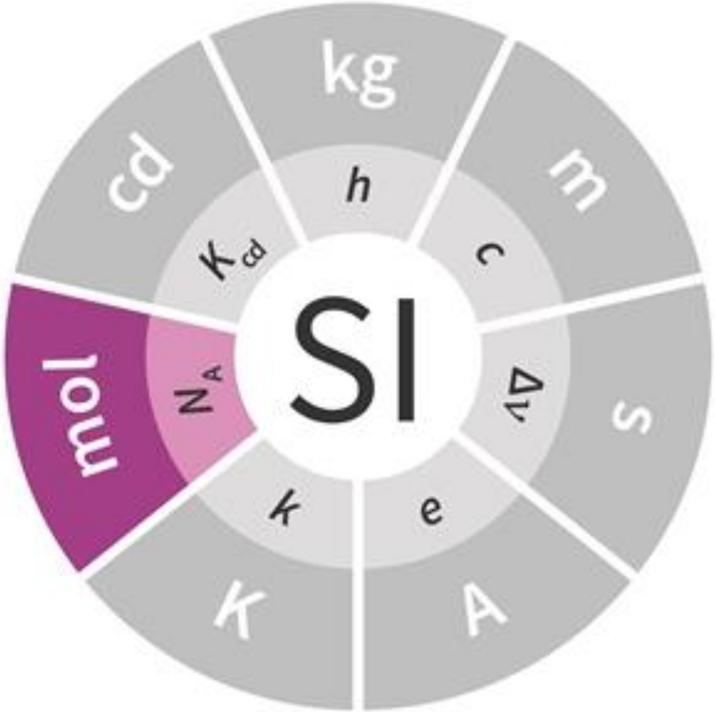
02 When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

03 The mole is a base unit of the Système International d'Unités.

DOI : 10.59161/CGPM1971RES3E

The mole: a brief history

Around early 1990 scientist began to propose a new paradigm to establish units of the SI based on fundamental constants.



The mole: a brief history

During the 21th CGPM celebrated in 2019, the new definition of the mol was establish:

SI base unit: mole (mol)

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

This definition implies the exact relation N_A = 6.022 140 76 x 10^{23} mol^{-1}. Inverting this relation gives an exact expression for the mole in terms of the defining constant N_A:

$$1 \text{ mol} = \frac{6.022\,140\,76 \times 10^{23}}{N_A}$$

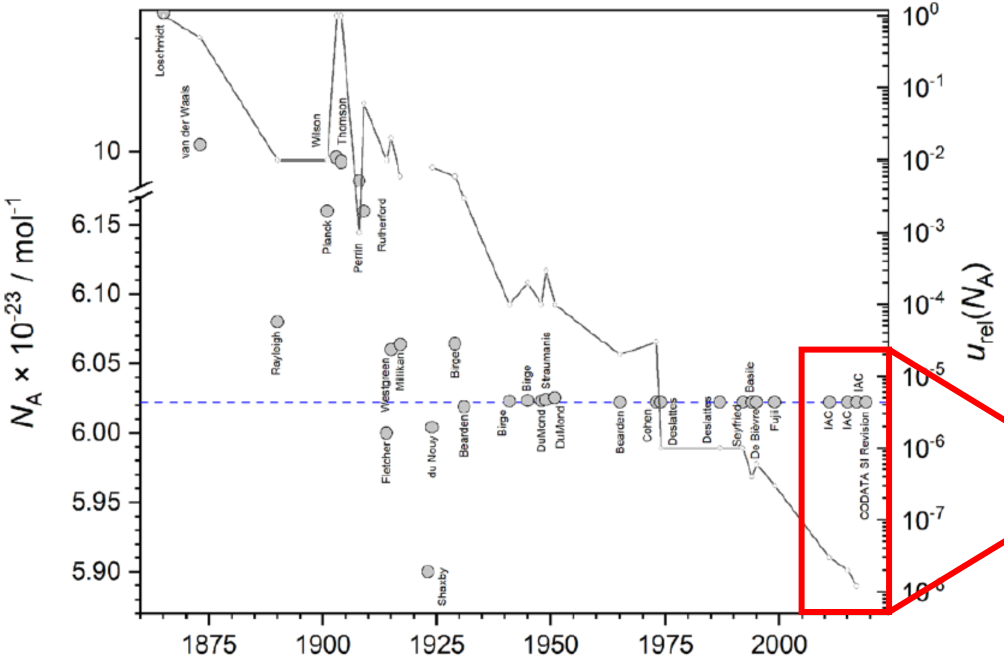
The effect of this definition is that the mole is the amount of substance of a system that contains 6.022 140 76 x 10^{23} specified elementary entities.

BIPM,2024

But, Where does this come from?

The mole: a brief history

Avogadro value (6.022 14076 x 10^{23}) was established from results coming from the International Avogadro Coordination (IAC) and NMJ-17 realization experiments.



- X-Ray Crystal Density (XRCD) method
- Method of least-squares (appendix E of CODATA-98)

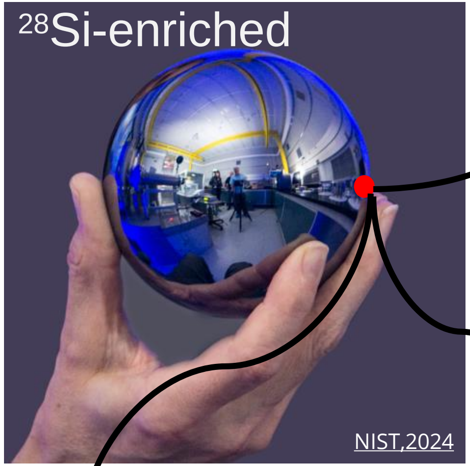
6.022 140 95(18) × 10^{23} mol^{-1}	3.0 × 10^{-8}	IAC-11
6.022 140 70(12) × 10^{23} mol^{-1}	2.0 × 10^{-8}	IAC-15
6.022 140 526(70) × 10^{23} mol^{-1}	1.2 × 10^{-8}	IAC-17
6.022 140 78(15) × 10^{23} mol^{-1}	2.4 × 10^{-8}	NMIJ-17

$$N_A = 6.022\,140\,758(62) \times 10^{23}\ \text{mol}^{-1}\quad [1.0 \times 10^{-8}].$$

Güttler, B., Rienitz, O., & Pramann, A. (2019). The Avogadro constant for the definition and realization of the mole. Annalen der Physik, 531(5), 1800292.
Mohr, P. J., Newell, D. B., Taylor, B. N., & Tiesinga, E. (2018). Data and analysis for the CODATA 2017 special fundamental constants adjustment. Metrologia, 55(1), 125-146.

The mole: a brief history

In a very simple way, the realization of the mole by the XRCD method can be described as follows:

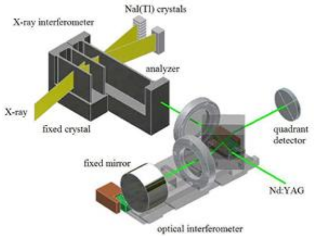


$$a_0 = \left(\frac{n}{\rho}\frac{M}{N_A}\right)^{\frac{1}{3}}$$

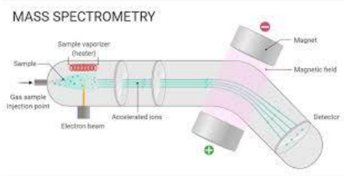
Bragg cristalography eq. (1913)

$$N_A = \frac{8}{a^3}\frac{M}{\rho} = \frac{8V}{a^3}\frac{M}{m}$$

optical sphere interferometer

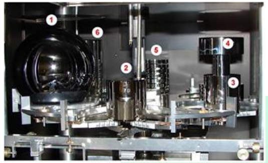


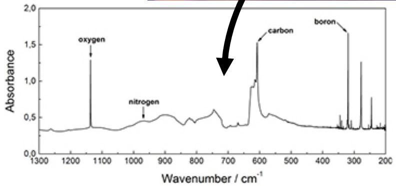
isotope ratio mass spectrometry



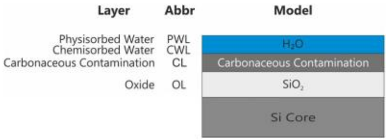
x-Ray interferometer

mass comparator at the 1 kg level





point defects



surface layers

Güttler, B., Rienitz, O., & Pramann, A. (2019). The Avogadro constant for the definition and realization of the mole. Annalen der Physik, 531(5), 1800292.
Fujii, K., Bettin, H., Becker, P., Massa, E., Rienitz, O., Pramann, A., ... & Borys, M. (2016). Realization of the kilogram by the XRCD method. Metrologia, 53(5), A19.
Becker, P. (2001). History and progress in the accurate determination of the Avogadro constant. Reports on Progress in Physics, 64(12), 1945.

The mole: a brief history

Next figure show the impact of the new definition:

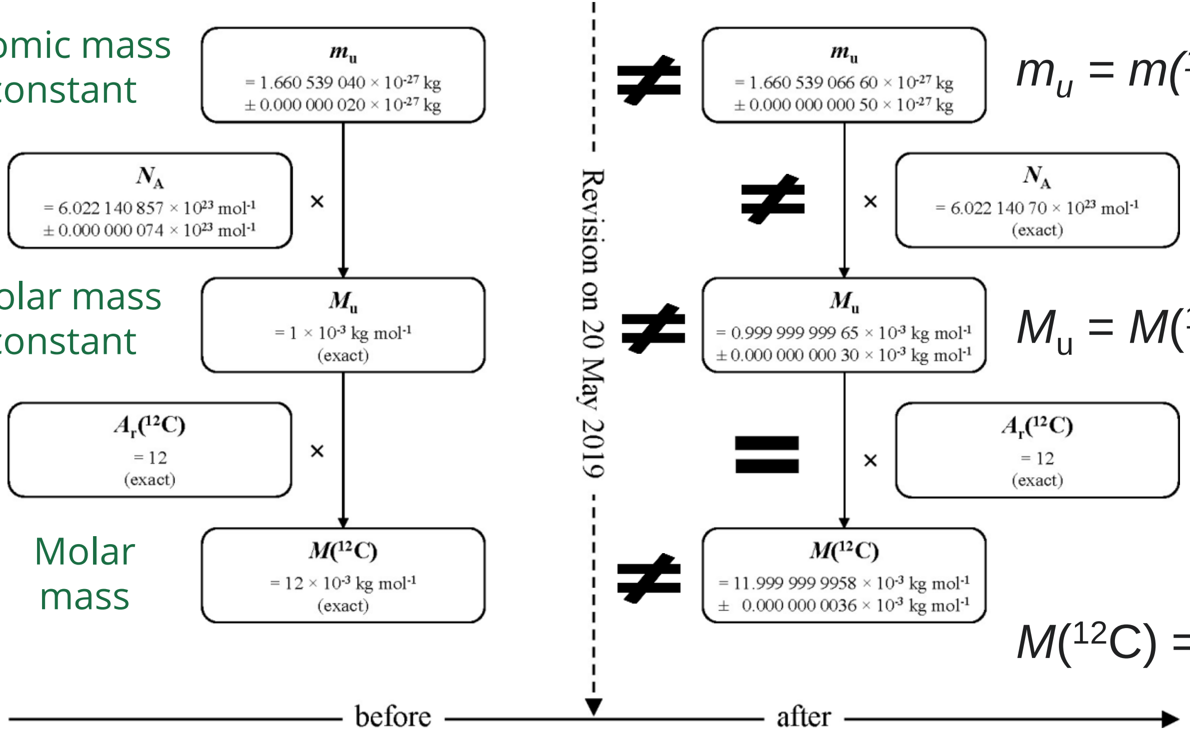
Atomic mass constant

Avogadro constant

Molar mass constant

Relative Atomic Mass of ^{12}C

Molar mass



$m_u = m(^{12}C)/12$

$M_u = M(^{12}C)/12$

$A_r(^{12}C) = m(^{12}C)/m_u$

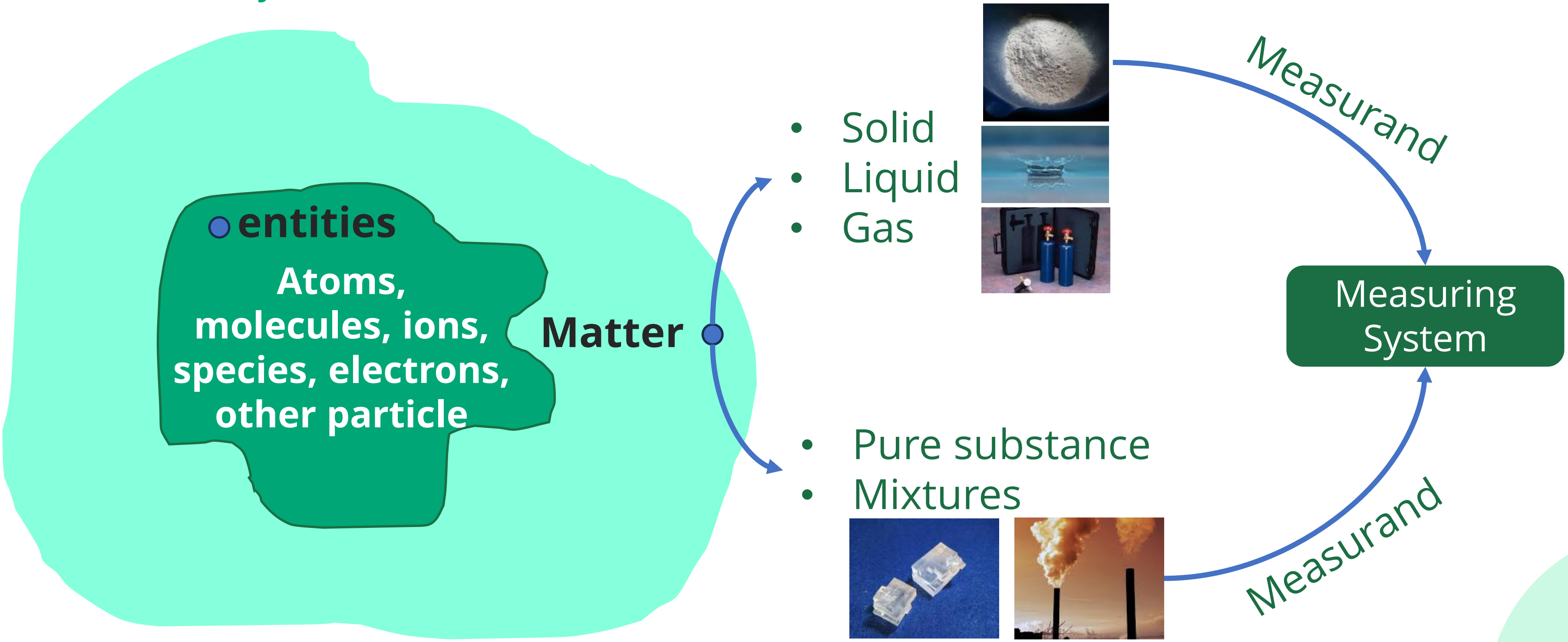
$M(^{12}C) = M_u \cdot 12$

Brown, R. J., Brewer, P. J., Pramann, A., Rienitz, O., & Güttler, B. (2021). Redefinition of the Mole in the Revised International System of Units and the Ongoing Importance of Metrology for Accurate Chemical Measurements.

Chapter 2: Basic measurement Principles in chemistry

Mesurand in Chemistry

Measurand in chemistry field have the same definition provide by VIM (2012): “Quantity intended to be measured” (VIM, 20212).



Mesurand in Chemistry

Measurand in chemistry field have the same definition provide by VIM (2012): “Quantity intended to be measured” (VIM, 20212).

Infant/Adult
Nutritional Formula
(milk/whey/soy-based)

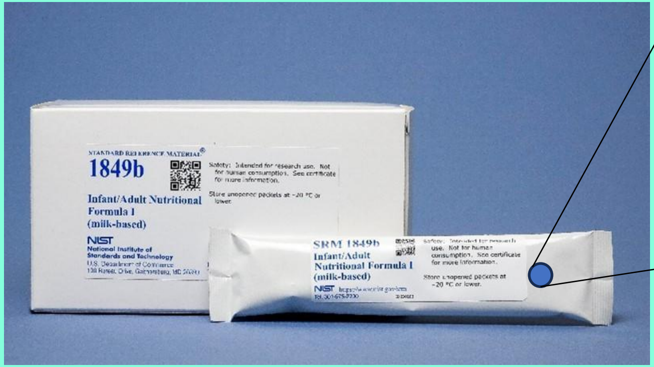


Table 1. Certified Values for Various Measurands in SRM 1869

	Mass Fraction[a] (mg/kg)
Calcium (Ca)	4560 ± 130
Copper (Cu)	19.00 ± 0.38
Chlorine (Cl)	5130 ± 130
Chromium (Cr)	0.859 ± 0.066
Iodine (I)	1.28 ± 0.15
Iron (Fe)	164.7 ± 3.7
Magnesium (Mg)	947 ± 10
Manganese (Mn)	46.0 ± 1.6
Molybdenum (Mo)	1.612 ± 0.047
Phosphorus (P)	4186 ± 57
Potassium (K)	7560 ± 110
Selenium (Se)	0.806 ± 0.083
Sodium (Na)	1877 ± 53
Zinc (Zn)	144.0 ± 3.2

	Mass Fraction[a] (mg/kg)
Ascorbic Acid (Vitamin C)	897 ± 43
Thiamine (Vitamin B_1)[b]	13.36 ± 0.32
Riboflavin (Vitamin B_2)	13.6 ± 1.5
Niacinamide (Vitamin B_3)	98.4 ± 2.2
Total Vitamin B_3 as Niacinamide	99.5 ± 4.4
Pantothenic Acid (Vitamin B_5)	64.9 ± 6.6
Pyridoxine (Vitamin B_6)[c]	13.09 ± 0.32
Cyanocobalamin (Vitamin B_{12})	0.0447 ± 0.0049
Biotin	1.89 ± 0.24
Total Choline[d]	1612 ± 64
Free Carnitine	103.5 ± 4.5

	Mass Fraction[a] (mg/g)
Cholesterol	0.1302 ± 0.0047

[a] Values are expressed as $x \pm U_{95\%}(x)$, where x is the certified value and $U_{95\%}(x)$ is the expanded uncertainty of the certified value. The true value of the analyte lies within the interval $x \pm U_{95\%}(x)$ with 95 % confidence. To propagate this uncertainty, treat the certified value as a normally distributed random variable with mean x and standard deviation $U_{95\%}(x)/2$ [2–6].
[b] Vitamin B_1 is reported as thiamine ion (265.36 g/mol), not thiamine chloride or thiamine chloride hydrochloride.
[c] Vitamin B_6 is reported as pyridoxine (169.18 g/mol), not pyridoxine hydrochloride.
[d] Choline is reported as the choline ion (104.17 g/mol).

NIST, 2024

Measuring system

In chemistry, measuring system typically encompass processes such as *identification, separation, isolation, purification, and quantification*, often utilizing one or more measuring instruments.

Nuclear Magnetic Resonance (NMR) Spectrometer	Inductively coupled plasma spectrometry (ICP-MS/OES)	Thermogravimetric Analyzer (TGA-MS/IR)	Transmission Electron Microscope (TEM-XPS/EDX)
UV-Vis/ NIR Spectrophotometer	Glow Discharge Spectrometer (GD-MS/OES)	Differential Scanning Calorimeter (DSC-MS/IR)	Atomic Force Microscope (AFM)
Fourier-Transform Infrared Spectroscopy (FTIR)	X-Ray Fluorescence Analyzer (XRF)	Karl-Fisher Coulometric/volumetric	Scanning Electron Microscope (TEM-XPS/EDX)
Gas Chromatography (GC-MS/FID/TCD/NPD/ECD)	Neutron Activation Analysis (NAA)	Coulometer	Analytical Balance (gravimetric)
Liquid Chromatography (LC-MS/DAD/UV/IR/IDMS)	Ion chromatography (IC)	Isotope Ratio Mass Spectrometer (IRMS)	Atomic Absorption Spectrophotometer (AAS)

Figures above represents some examples of common measuring instrument used in the chemical metrology.

Metrological Traceability in Chemistry

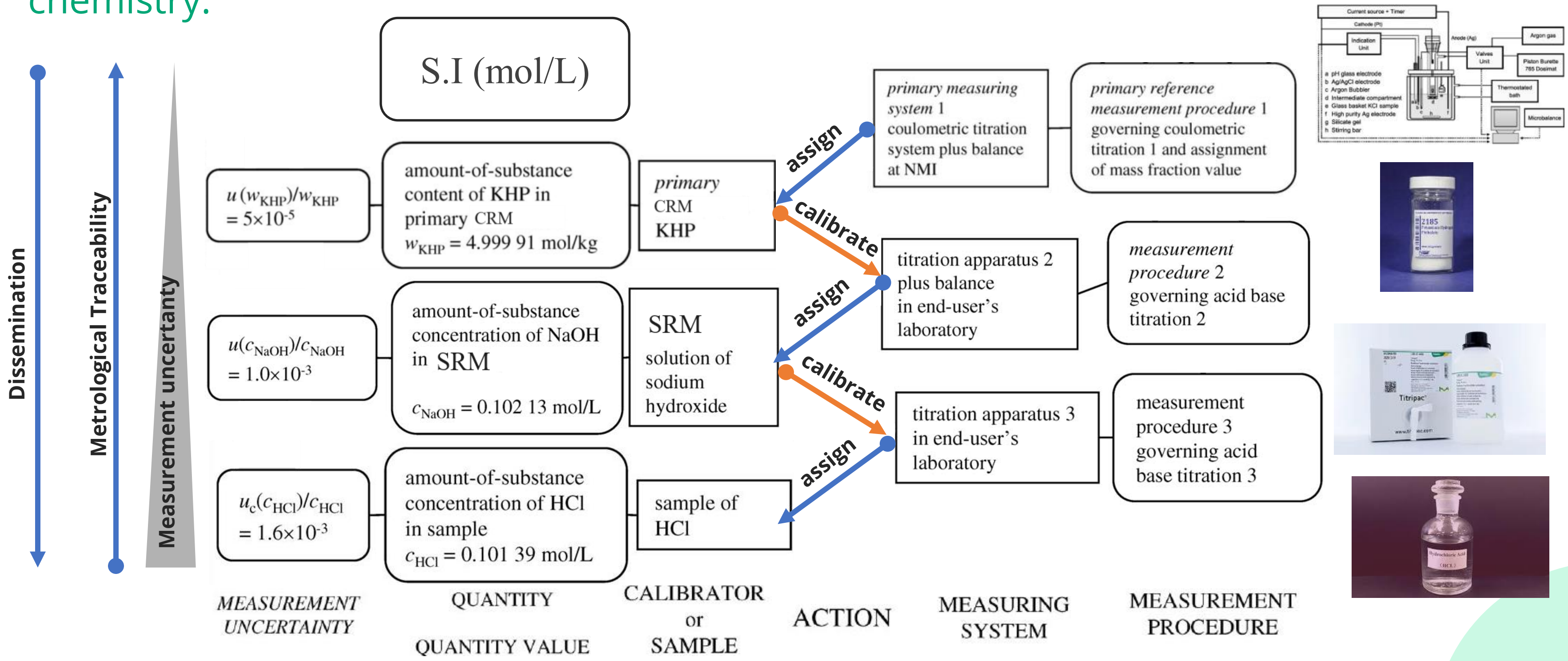
Metrological traceability in chemistry refers to the chain of calibrations and measurements that link the results of an analysis to a reference standard (S.I):

Dissemination ↓

1	International System of Units (SI)	Amount of Substance (Mol)	CGPM/BIPM
2	Primary Reference Materials (PRMs)	Certified reference materials (CRMs) with the highest metrological quality, directly traceable to SI units.	NMIs
3	Secondary Reference Materials (SRMs)	Reference materials produced from PRMs. Used for calibration of instruments or validation of methods in laboratories	NMI or DI
4	Calibration services	Laboratories that use SRMs to calibrate measurement instruments and ensure their results are traceable to national standards.	Metrology Laboratory (Secondary)
5	Measurement services	Laboratories that perform routine chemical analyses, using calibrated instruments and validated methods to ensure traceability.	Analytical Laboratories(accredited)
6	Industrial Measurement	Laboratories that perform quality control (QC) analysis or verification of products and raw materials	Industrial Laboratories

Metrological Traceability in Chemistry

The figure below provides a practical illustration of metrological traceability in chemistry:

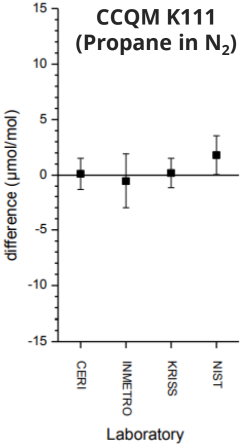


Adapted from: [De Bièvre, P., Dybkaer, R., Fajgelj, A., & Hibbert, D. B. (2011). Metrological traceability of measurement results in chemistry: Concepts and implementation (IUPAC Technical Report). Pure and applied chemistry, 83(10), 1873-1935.]

Chapter 3: Structure of the CCQM and main focus areas

Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology (CCQM)

The CCQM is responsible for developing, improving and documenting the equivalence of national standards (CRM and reference methods) for chemical and biological measurements.



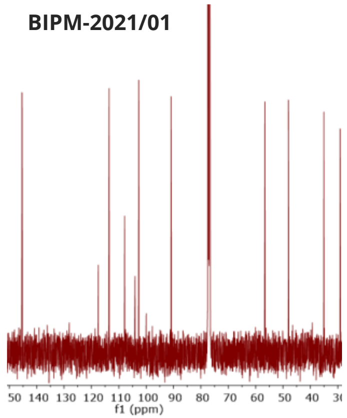


Figure 3 – ^{13}C NMR spectrum of AfB_1 in $CDCl_3$.

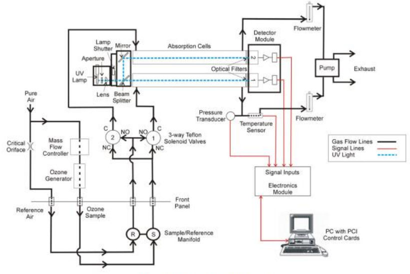
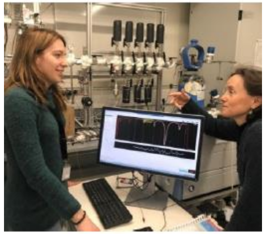


Figure 1. Schematic of the SRP system.



Calibration service: Ozone photometers

Absolute expanded uncertainty (k = 2) / (nmol/mol)
2 Q[0.52, 0.0034 $x(O_3)$, 0.0106 $x(O_3)$]

- Establish global comparability of measurement
- Contribute to global measurement standards, methods and facilities (Chem & Bio)
- Contribute to the implementation and maintenance of the CIPM MRA (Chem & Bio)
- Review and advise the CIPM on the u(xi) of the BIPM's measurement services
- Act as a forum for the exchange of information

Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology (CCQM)

Also, the CCQM is organized in 12 different working groups that cover most of the chemical and biological measurements:

Working Groups

To review, advice and provide information on the mol	CCQM-AH-WG-MOLE CCQM *AD HOC* WORKING GROUP ON THE MOLE	CCQM-CAWG CCQM WORKING GROUP ON CELL ANALYSIS	Cellular attribute (Count, structure Morfology, biomarkers)
pH, Conductivity, KCl purity	CCQM-EAWG CCQM WORKING GROUP ON ELECTROCHEMICAL ANALYSIS	CCQM-GAWG CCQM WORKING GROUP ON GAS ANALYSIS	CO_2, CH_4, CO, NO, N_2
As, Pb, Cd, Hg, Na, Ca, Cu	CCQM-IAWG CCQM WORKING GROUP ON INORGANIC ANALYSIS	CCQM-IRWG CCQM WORKING GROUP ON ISOTOPE RATIOS	$\delta^{13}C$ (in Vainillin) $\delta^{13}C$ (in Honey)
Generated guidance documents on the CIPM MRA	CCQM-KCWG CCQM WORKING GROUP ON KEY COMPARISONS AND CMC QUALITY	CCQM-NAWG CCQM WORKING GROUP ON NUCLEIC ACID ANALYSIS	Genomic DNA fragments
AfB_1, Uric Acid, Bisphenol A	CCQM-OAWG CCQM WORKING GROUP ON ORGANIC ANALYSIS	CCQM-PAWG CCQM WORKING GROUP ON PROTEIN ANALYSIS	Purity in peptides
Specific Adsorption (BET) in nanoporous Al_2O_3	CCQM-SAWG CCQM WORKING GROUP ON SURFACE ANALYSIS	CCQM-SPWG CCQM STRATEGIC PLANNING WORKING GROUP	

BIPM-CCQM,2024

Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology (CCQM)

Also, the CCQM have task groups to support and develop specific projects or developments in the field of chemistry and biology:

Task Groups

CCQM-TG-FOOD
CCQM TASK GROUP ON FOOD MEASUREMENT
(Food security and food safety)

CCQM-TG-LI-ION
CCQM TASK GROUP ON ON METROLOGY FOR LI-ION BATTERIES
(Li-ion technology)

CCQM-TG-PANDEMIC
CCQM TASK GROUP ON INFECTIOUS DISEASE DIAGNOSTICS AND METROLOGY FOR PANDEMIC PREPAREDNESS
(Metrology of infectious disease diagnostics)

CCQM-TG-KCRV
CCQM TASK GROUP ON GUIDANCE FOR THE ESTIMATION OF A CONSENSUS
(Review and update CCQM guidance)

CCQM-TG-NMMS
CCQM TASK GROUP ON NANO- AND MICROPLASTICS MEASUREMENTS AND STANDARDS
(explore potential activities in this field)

CCQM-TG-STAKEHOLDER
CCQM TASK GROUP ON STAKEHOLDER ENGAGEMENT
(Tasks Completed)

BIPM-CCQM, 2024

Chapter 4: SIM MW-08 perspective

RMO in America (SIM)

The Inter-American Metrology System (SIM) is the regional organization of metrology in America

Promote international cooperation on metrology issues and is committed to implementing a global measurementsystem that all users can trust.

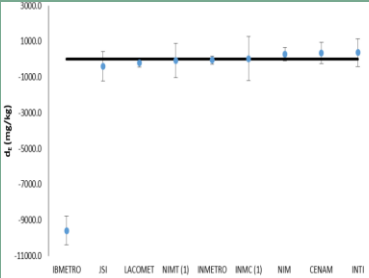
Promotes and supports an integrated measurement infrastructure in the Americas.

KCDB	SIM
Number of CIPM MRA participants	56
Number of CMCs	4538
Number of key comparisons	78
Number of supplementary comparisons	124

MWG-8 in CHEMISTRY & BIOLOGY (SIM)

The Chemical Metrology Working Group in SIM, MWG-8, supports SIM and its member NMIs/DIs in reaching the obligations requirements of CIPM-MRA in the field of metrology in chemistry and biology measurements

Organizes regional key and supplementary comparisons as well as pilot studies linked to the CCQM



Facilitates **cooperation in preparing, reviewing, publishing and maintaining CMCs** claims of member economies and DIs

KCDB SIM

Number of CIPM MRA participants	56
Number of CMCs	4484
Number of key comparisons	78
Number of supplementary comparisons	122

Disseminates knowledge and facilitates technical cooperation through meetings, workshops, awareness seminars and training opportunities

Seeks harmonization among its members through sustainable **networking**

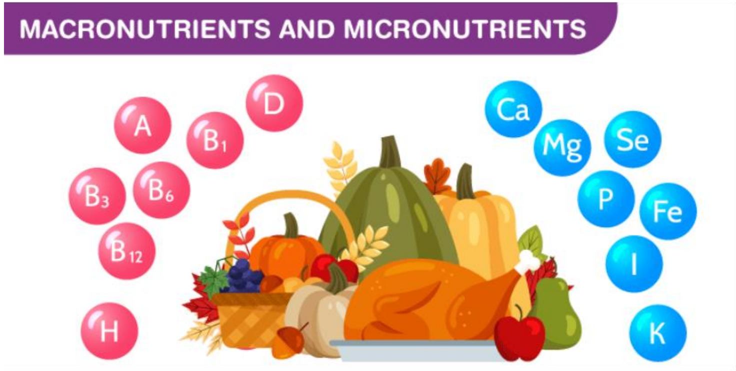
SIM MWG-8 comparisons (in progress and finished)

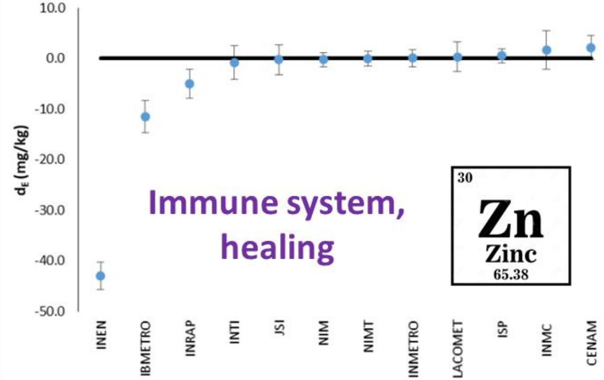
K-comparisons ensure comparability between different economies and serve as fundamental evidence to enhance safety and health in SIM countries

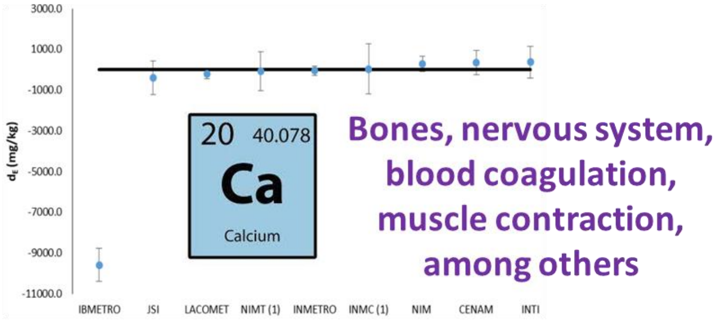
Field	Pilot Lab	Name	Measurement Capability	Status	Number participants
OA	CENAM/INMETRO	SIM.QM-S17	Ethanol in Water	Draft B (set to OQWG)	13
IA	NRC	SIM.QM-S10	Trace Elements in Skim Milk Powder	KCDB (Published on)	12
	LATU	SIM.QM-S11&P25	Trace of As, Cd, P and Na in Mate	Draft A (presented to IAWG)	16
	NRC	SIM.QM-S12	Elements in Natural Water	Draft A (presented to IAWG)	21
	CENAM/INMETRO	SIM.QM-S13	Elements in Cu Concentrate & Ore	Draft B (on discution)	11
	INMETRO	SIM.QM-S16	Metals in Water	Running	>10
GA	CENAM-KRISS	SIM.QM-S5	Natural Gas	Draft A (waiting aproval GAWG)	7
	CENAM-KRISS	SIM.QM-S6	Automotive Emissions	Draft A (available April 2023)	5
	INMETRO	SIM.QM-S9	Biogas	Draft B (available April 2023)	4
	CENAM	SIM.QM-S14	Carbon Dioxide in Nitrogen	Draft A (available March 2023)	4
	CENAM	SIM.QM-S15	Methane in Air	Draft B (available March 2023)	4
NA	CENAM	SIM.QM.Pilot study	SARS-CoV-2 DNA Copy number quantification	Draft A (Report prepared)	4

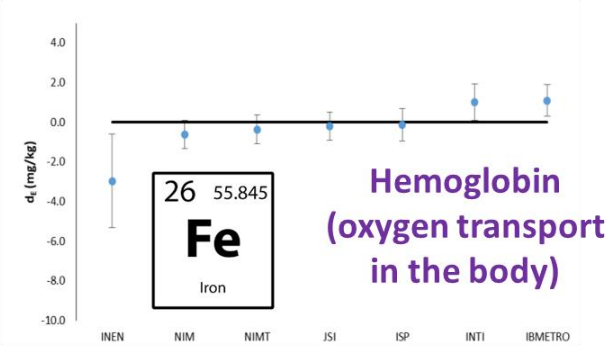
SIM MWG-8 comparisons (in progress and finished)

K-comparisons ensure comparability between different economies and serve as fundamental evidence to enhance safety and health in SIM countries









SIM.QM-S10 **Trace Elements in Skim Milk Powder** Metrologia (2021) 58.1A, 08008

SIM MWG-8 comparisons (in progress and finished)

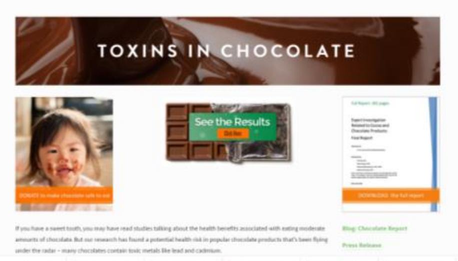
K-comparisons ensure comparability between different economies and serve as fundamental evidence to enhance safety and health in SIM countries

Chocolate (final Product)

Global chocolate consumption:
~7 500 million kg/year
Global chocolate industry worth:
~ USD $130 billion

Cacao (primary ingredient in chocolate making)

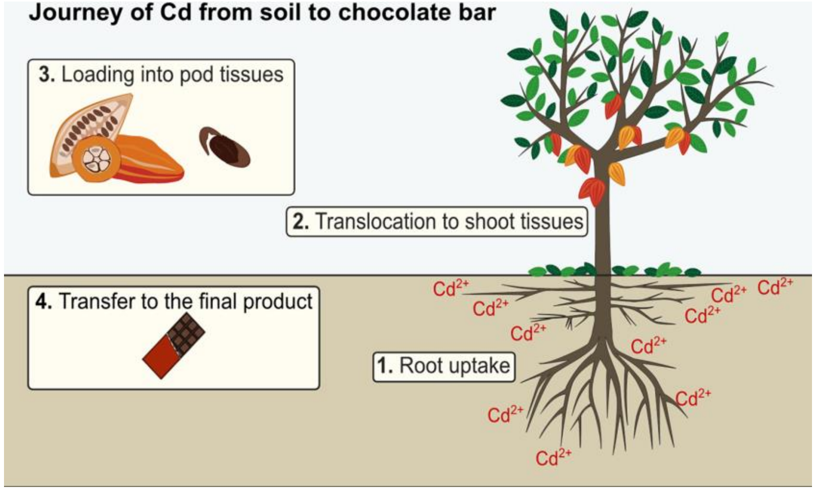
Global Production:
~ 5 000 million kg/year



Field	Pilot Labs	Comparison type	Measurement Capability	Status
IA	NRC & CENAM	Supplementary	Cd and Pb in Cacao powder	• Presented at IAWG (2023) • Running in 2024

SIM MWG-8 comparisons (in progress)

K-comparisons ensure comparability between different economies and serve as fundamental evidence to enhance safety and health in SIM countries



Science of the Total Environment (2021) 781, 146779

Regulatory frameworks	Cd	Pb
EU Regulations (488/2014) cocoa powder	**0.60 mg/kg**	--
FAO/ WHO food standards programme (Codex alimentarius commission)	under revision	
California Proposition 65	4.1 µg/day	0.5 µg/day
US FDA guidance for industry		0.1 mg/kg

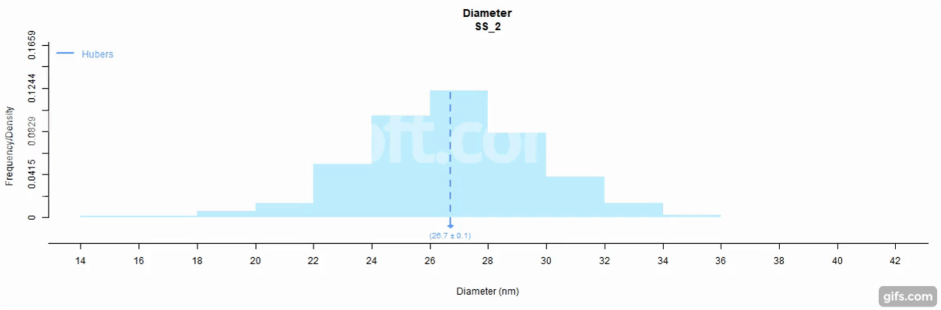
Field	Pilot Labs	Comparison type	Measurement Capability	Status
IA	NRC & CENAM	Supplementary	Cd and Pb in Cacao powder	• Presented at SIM MWG8 (September 2022) • Presented at IAWG (2023)

SIM Dissemination projects and training

Metrological dissemination activities, as well as trainings and workshops that the SIM has either participated in or plans to organize in the near future

Workshop "Making an impact on water quality for public health & safety:

- ✓ Held from March 6 to 9, 2023, in Kuala Lumpur, Malaysia
- ✓ Participation of 3 representatives from SIM NMIs



NanoWorkshop (PROPOSAL)

- ✓ Confirmed participants (8 participants or more):
- ✓ Costa Rica (LACOMET), Mexico (CENAM), Brazil (INMETRO), Argentina (INTI), Uruguay (LATU), Colombia (INM Colombia), Chile (CODELCO) and Peru (INDECOPI).
- ✓ Workshop would be an activity attached to the 2025 annual meeting of the SIM MWG-8 Chemistry.

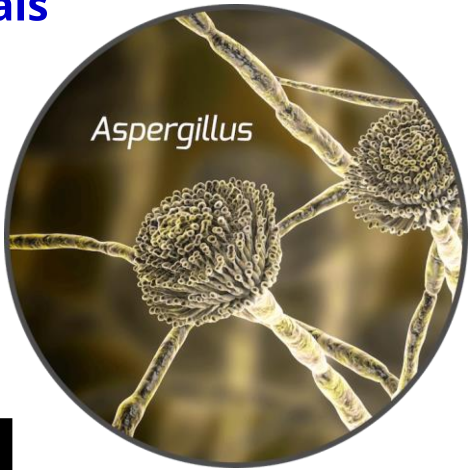
SIM Dissemination projects and training

Other metrological dissemination activities, as well as trainings and workshops that the SIM has vinculated.

Capacity Building and Knowledge Transfer Programme

Safe Food and Feed – Mycotoxin calibrant reference materials

Developing Capabilities → Transfer of knowledge → Applying knowledge → Demostration Competence → Providing Services



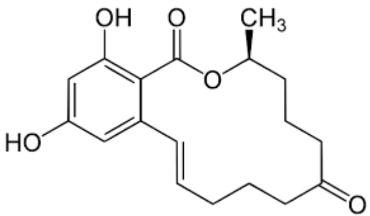
SIM Dissemination projects and training

Other metrological dissemination activities, as well as trainings and workshops that the SIM has vinculated.

CBKT Capacity Building and Knowledge Transfer Programme

Safe Food and Feed – Mycotoxin calibrant reference materials

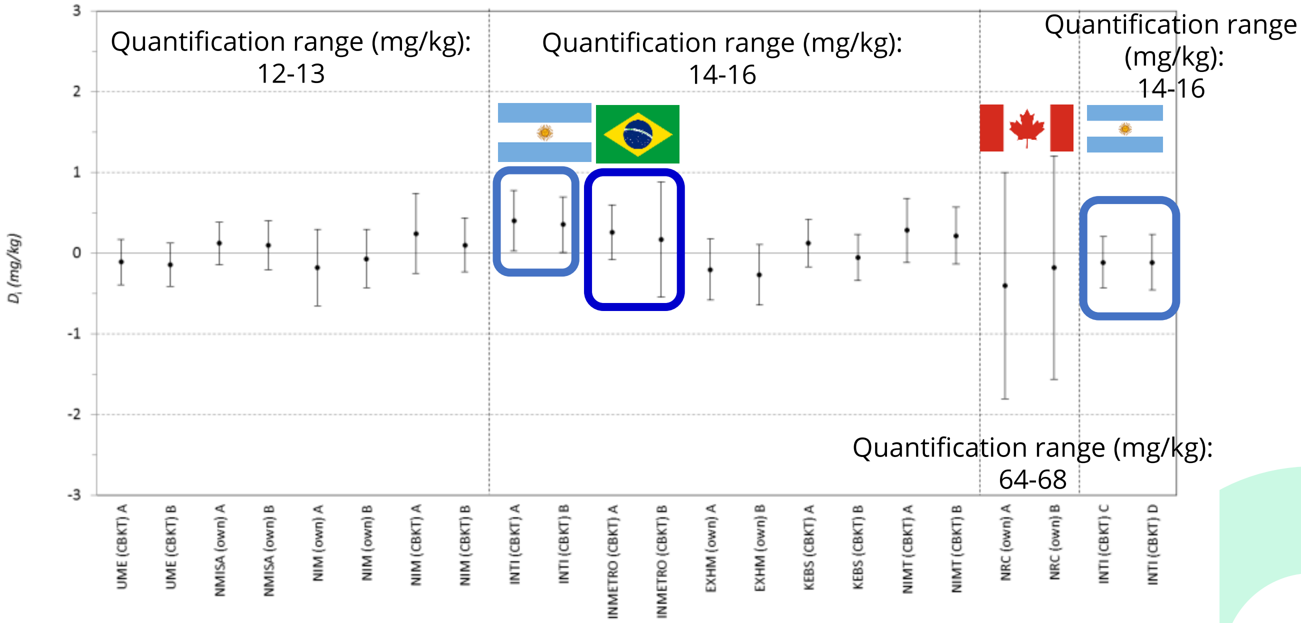
Demostration Competence



trans-ZEN

toxin that binds to estrogen receptors, causing infertility, abortion or other breeding problems

trans-zearalenone (trans-ZEN) in acetonitrile (ACN)



Chapter 5: Current technical challenges and future trends

Current technical challenges and future trends

Finally, as science is always in constant evolution, there still technical challenges and future trends to achieve in this field. Some examples for specific CCs are:

CCQM-IAWG

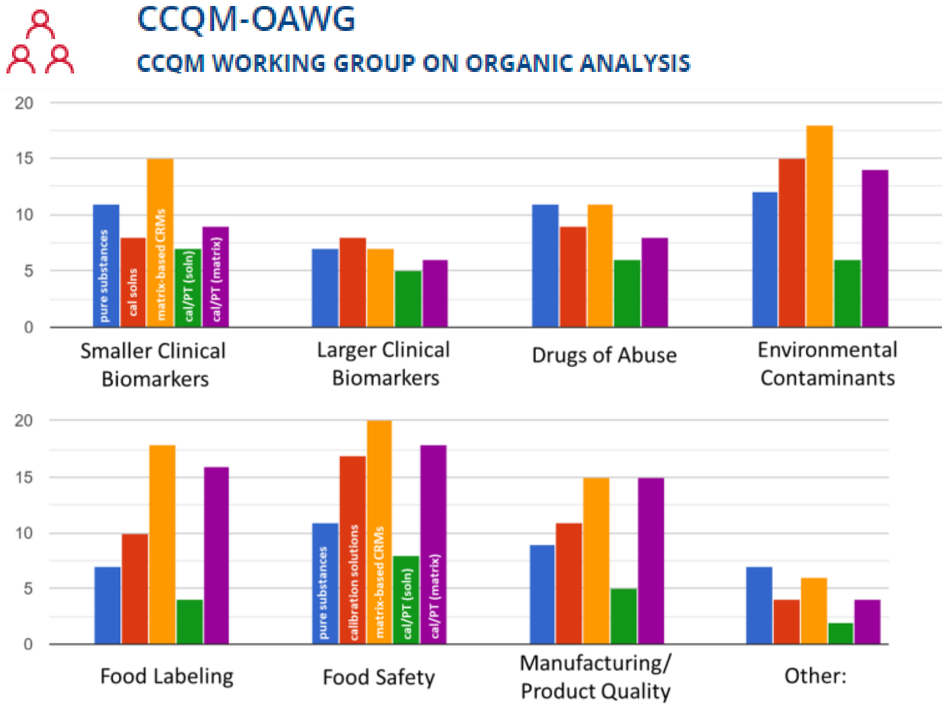
CCQM WORKING GROUP ON INORGANIC ANALYSIS

- **Metrological traceability to the SI.** Reliable purity assays can be quite challenging, assays include the most appropriate treatment of **nondetectable elements** (assymetric $u(x_i)$)
- **Nanoparticle metrology.** Reliable, practical, and affordable measurement **methods for nanoparticles are often unavailable**.
- **Element-based quantitation of biomolecules.** **Reliable measurements of biomolecules**, such as proteins, peptides, nucleotides, DNA, and RNA are of great important to the medical and biotechnology fields.
- **Small sample and spatially-resolved metrology.** **IAWG has had no KCs or PSs on these topics**, even though this type of metrology is extremely important in forensics, electronics, biology, and a host of other fields (laser ablation).
- **Elemental speciation.** **There is still a need for further IAWG work**.

IAWG Strategy document

Current technical challenges and future trends

Finally, as science is always in constant evolution, there still technical challenges and future trends to achieve in this field. Some examples for specific CCs are:



[OAWG Strategy document]

Priority services for OAWG members across sectors. Services include: (**blue**) pure organic calibration materials, (**red**) solution calibration materials, (**orange**) matrix-based reference materials, (**green**) calibration/PT services for chemical purity and calibration solutions, and (**purple**) calibration/PT services for matrix-based measurements.

Current technical challenges and future trends

Finally, as science is always in constant evolution, there still technical challenges and future trends to achieve in this field. Some examples for specific CCs are:

CCQM-SAWG

CCQM WORKING GROUP ON SURFACE ANALYSIS

- **Accurate measurement of in thin films, layers and coatings from atomic layers.** For example, establishing **traceability for compositional measurements of homogeneous thin films**.
- **Develop metrological understanding of methods used to map or image chemistry.** For example, a pilot study on **Raman microscopy**.
- **Element-based quantitation of biomolecules.** Reliable measurements of biomolecules, such as proteins, peptides, nucleotides, DNA, and RNA are of great important to the medical and biotechnology fields.
- **Metrology of nanostructured and highly porous materials.** Create infrastructure for the chemical measurement for this **new materials** and maintaining and building upon gas sorption measurements.
- **Support the development of chemical metrology for nanoparticles.** For example, **AuNPs concentration with IAWG**.

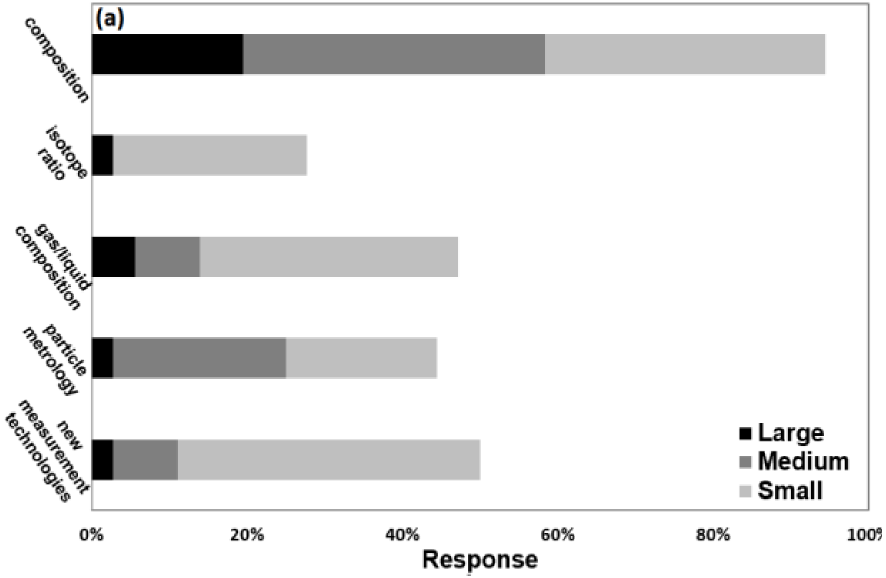
SAWG Strategy document

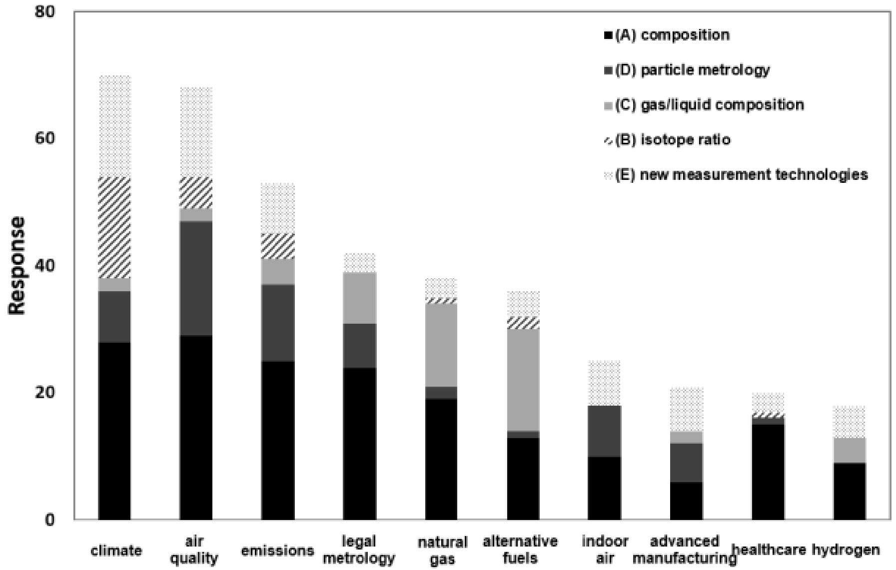
Current technical challenges and future trends

Finally, as science is always in constant evolution, there still technical challenges and future trends to achieve in this field. Some examples for specific CCs are:

CCQM-GAWG

CCQM WORKING GROUP ON GAS ANALYSIS





Institute's programme size and future projection (a) against five measurement capabilities. Application of the five measurement capabilities against the sectors described, as indicated by the GAWG strategy survey participants

GAWG Strategy document

SIM
SISTEMA INTERAMERICANO DE METROLOGÍA

SIM METROLOGY SCHOOL

Thanks!

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