Title: New strategies to establish and disseminate SI traceability for isotope ratios, the kilogram and the mole

Abstract

Isotope ratio data are used for many purposes including the determination of molar masses of multi-isotopic elements with applications in sectors such as forensics, food fraud and climatology. Isotope ratios directly impact the redefinition of the kilogram and mole SI base units. With a redefinition of these base units, new strategies are required for new primary isotope reference materials, whose isotope ratios are traceable to the SI. This in turn will ensure the comparability of isotope ratio data. Proposals are invited to develop such new procedures for the key elements S, Si, Ca, Sr and Nd at relative uncertainty levels of ≤ 0.01 %.

Keywords

SI base units, traceability, isotope ratio measurement, atomic weight, molar mass, primary isotope standards, synthetic isotope mixtures, isotope ratio variation, mass fractionation

Background to the Metrological Challenges

The determination of isotope ratios represents a key issue for challenging measurements in many fields of science and technology including meteorology/climatology, geo- and cosmo-chemistry and oceanography, which affect crucial progress in applications such as climate change research and food safety surveys.

Despite the importance of these measurement results and considerable efforts in the past, SI-traceable measurement results remain a critical and highly demanding task in all the areas mentioned above. This has caused the *Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology* (CCQM) to request a “traceability exception related to delta scale isotope ratio measurements” from the *International Committee for Weights and Measures* (CIPM). Such delta scale measurements in most cases are currently based on artefacts (known as isotope reference materials or iRMs) of arbitrarily selected materials without SI-traceable isotopic composition, or a sufficiently small measurement uncertainty to fulfil the needs arising from recent applications. Many materials are provided in solid form and the inhomogeneity of solid materials, which often are due to technical purification processes such as zone refining, can reach levels close to the natural isotopic variation of the corresponding element, rendering such materials unsuitable for current isotope research. Additionally, currently used reference materials are running out of stock or are even lacking for a number of elements.

Primary isotope ratio measurement results for these systems with relative measurement uncertainties of ≤ 0.01 % are urgently needed to overcome these challenges. The target elements sulphur (S), silicon (Si), calcium (Ca), strontium (Sr) and neodymium (Nd) are particularly important, because they span a wide range of scientific fields, they cover different measurement techniques and they offer a large number of applications and routinely performed isotope ratio measurements. New approaches to measuring isotope ratios without the use of iRMs, such as those based on virtual element isotope dilution mass spectrometry (VE-IDMS) and high-resolution continuum source molecular absorption spectrometry (HR-CS-MAS), have been proposed and their potential must be assessed and disseminated to enable the European metrology network (including NMIs and DIs) to improve their calibration services.

Objectives

Proposers should address the objectives stated below, which are based on the PRT submissions. Proposers may identify amendments to the objectives or choose to address a subset of them in order to maximise the overall impact, or address budgetary or scientific / technical constraints, but the reasons for this should be clearly stated in the protocol.

The JRP shall focus on the traceable measurement and characterisation of isotope ratios targeting the isotopic systems sulphur (S), silicon (Si), calcium (Ca), strontium (Sr) and neodymium (Nd)..

The specific objectives are

1. To calibrate mass spectrometric measurements of elements with four or more isotopes, such as Ca and Nd, at relative uncertainties of ≤ 0.01 %. To develop new analytical procedures for this purpose and validate them through comparison with currently used semi-empirical approaches.
2. To determine the molar mass of Si with a close to natural isotopic composition, with measurement uncertainties in the order of 10^{-7} or better. To develop, test and validate new mathematical and experimental approaches for this purpose, for example based on the VE-IDMS method.
3. To model and evaluate instrumental mass fractionation, which enables SI traceable isotope ratio measurements without the need for an isotope reference material (iRM) of the same element. Target isotope systems to be S, Si, Ca, Sr and Nd.
4. To develop new procedures for measuring SI traceable isotope ratios of Si, Ca, Sr and Nd without the use of iRMs, for example by applying the recently introduced high-resolution continuum source molecular absorption spectrometry (HR-CS-MAS) method. Proposals should consider the applicability of other optical techniques such as laser ablation molecular isotopic spectrometry for absolute isotope ratio measurements.
5. To facilitate the take up of the technology and measurement infrastructure developed in the project by the measurement supply chain (European reference material producers, European and International metrology organisations), standards developing organisations (IUPAC, IAEA, ISO) and end users (such as medical, forensic and food scientists).

These objectives will require large-scale approaches that are beyond the capabilities of single National Metrology Institutes and Designated Institutes. To enhance the impact of the research work, the involvement of the larger community of metrology R&D resources outside Europe is recommended. A strong industry involvement is expected in order to align the project with their needs and guarantee an efficient knowledge transfer into industry.

Proposers should establish the current state of the art, and explain how their proposed project goes beyond this.

EURAMET expects the average EU Contribution for the selected JRPs in this TP to be 1.8 M€, and has defined an upper limit of 2.1 M€ for this project.

EURAMET also expects the EU Contribution to the external funded partners to not exceed 20 % of the total EU Contribution across all selected projects in this TP.

Potential Impact

Proposals must demonstrate adequate and appropriate participation/links to the "end user" community, describing how the project partners will engage with relevant communities during the project to facilitate knowledge transfer and accelerate the uptake of project outputs. Evidence of support from the "end user" community (e.g. letters of support) is also encouraged.

You should detail how your JRP results are going to:

- Address the SRT objectives and deliver solutions to the documented needs,
- Feed into the development of urgent documentary standards through appropriate standards bodies,
- Transfer knowledge to the geochemical, food, forensics and health sectors.

You should detail other impacts of your proposed JRP as specified in the document "Guide 4: Writing Joint Research Projects (JRPs)"

You should also detail how your approach to realising the objectives will further the aim of EMPIR to develop a coherent approach at the European level in the field of metrology and include the best available contributions from across the metrology community. Specifically, the opportunities for:

- improvement of the efficiency of use of available resources to better meet metrological needs and to assure the traceability of national standards
- the metrology capacity of EURAMET Member States whose metrology programmes are at an early stage of development to be increased
- organisations other than NMIs and DIs to be involved in the work

Time-scale

The project should be of up to 3 years duration.