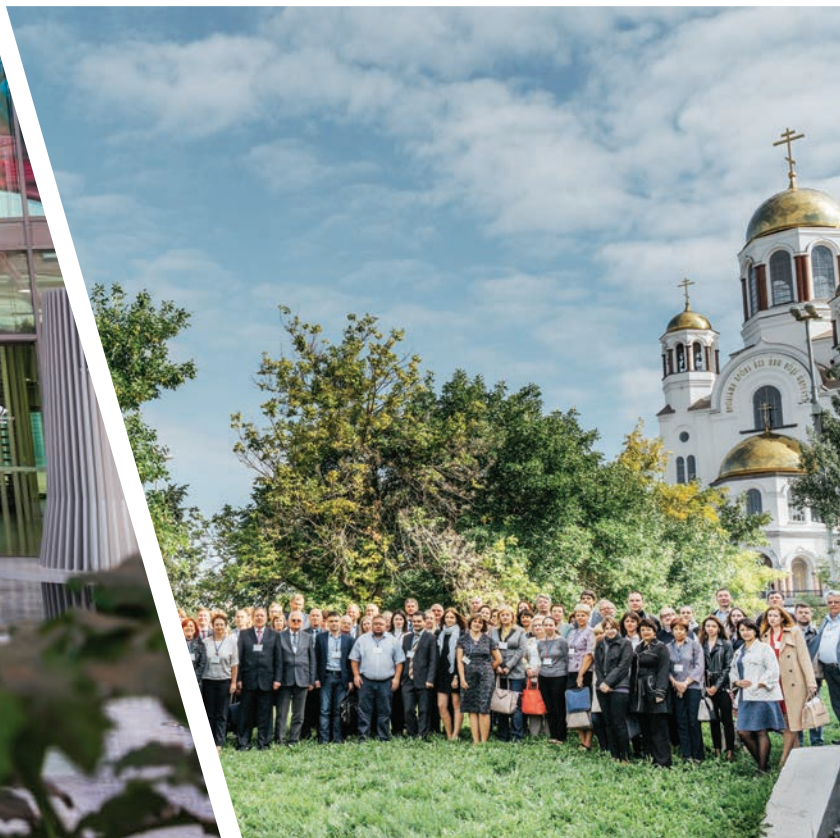
CITAC
Cooperation on International Traceability in Analytical Chemistry

CITAC NEWS

APRIL 2019



FOREWORD BY THE CHAIR

2018 IS A YEAR OF CHANGE

Michela Sega // INRIM Italy

2018 was a special year for the international chemical community. The decision taken at the 26th General Conference on Weights and Measures in November on the redefinition of the New SI, which will link the definition of the mole to a fundamental constant, i.e. the Avogadro constant, represents a revolutionary paradigm shift. This important change in terms of perspective does not mean that the mission of CITAC of promoting the metrological traceability of chemical measurements at the worldwide level has come to an end. The redefinition of SI will be a starting point towards new challenges and new goals to be faced. In addition, the proactive involvement of CITAC will be fundamental in disseminating the new concept, reassuring the chemical community that the big change must nevertheless guarantee the continuity in the everyday life and in the metrological traceability approach.

In 2018, new projects have started within the cooperation of CITAC with other International Organisations. A new Joint EURACHEM/CITAC Working Group on Reference Materials was established. It is coordinated by Marina Patriarca (Italy), who was elected as EURACHEM chair in May 2018, during the EURACHEM General Assembly. The Working Group is currently carrying out the revision of the EURACHEM Guide "Selection and use of reference materials (2002)", in order to promote the dissemination of good practice in this field at the European and international level. In 2018 a EURACHEM/CITAC leaflet "Setting Target Measurement Uncertainty" was also published. On the site of the cooperation with IUPAC, the IUPAC project n. 2018-004-1-500 "IUPAC/CITAC Guide for evaluation of risks of conformity assessment of a multicomponent material or object due to measurement uncertainty" has started in July 2018. It aims at preparing a guide which will be helpful to improve the understanding of the consequences of measurement uncertainty and correct choice of methods for testing chemical composition of multicomponent materials and objects.

2018 saw also the birth of a new CITAC logo, which still embodies the concept of the metrological traceability pyramid in a new guise.

I would like to spend also some words to congratulate the Winners of CITAC Best Paper Award 2017, authors of important and innovative papers in the field of metrology in chemistry, who presented their work in the 33rd CITAC meeting held in Sèvres on 21st April 2018: Dr. Marco Di Luzio, INRIM, Italy, and his coauthors in *Anal. Chem.* 89 (2017) 6726-6730; Adriaan M.H. van der Veen, VSL, The Netherlands, in *Accred. Qual. Assur.* 22 (2017) 1-3 ; Dr. Jun Wang, NIM, China, and her coauthors in *Anal. Chem.* 89 (2017) 9031-9038. According to the best

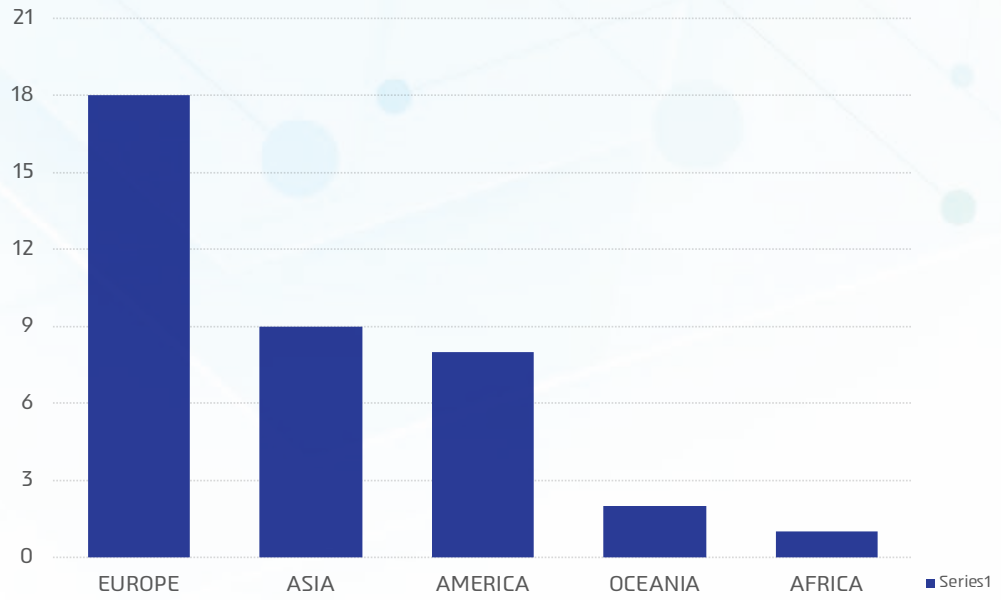


Fig. 1: Geographical distribution of CITAC members

CITAC tradition, the three papers are related to different innovative issues and the presentation of the works raised interesting discussions during the meeting.

In the past two years, new members joined CITAC, bringing new skills and competencies and a lot of enthusiasm. I would like to give a special warm welcome to Dr. Paola Fisicaro (France), Prof. Tony Rogério de Lima Dadamos (Brasil), Dr. Jorge Eduardo de Souza Sarkis (Institute of Energy and Nuclear Research, Brazil) and Dr. Narine Oganyan (VNIIFTRI) who joined CITAC family in 2018.

Due to this new memberships, at present CITAC counts 38 members, coming from all the continents. Figure 1 reports the geographical distribution of the memberships.

There are still some areas in the world where the involvement in CITAC needs to be further promoted in order to fulfill our primary mission. I am confident that the process we have started will give successful results in the near future.

ADDRESS OF THE VICE-CHAIR

Bernd Güttler // Physikalisch-Technische, Bundesanstalt (PTB), Germany

It is now ten years ago that EURAMET, the European Association of National Metrology Institutes, started its first own research programme – iMERA-plus. The current version is called European Metrology Programme for Innovation and Research (EMPIR). It fosters the research collaboration among the metrology institutes in Europe and provided, for the first time, financial support for joint research in metrology. Metrology in chemistry in Europe had a considerable share in these programmes, especially in the targeted programmes for environment, health and energy but also in other sections. After a decade of such joint activities under the auspices of EURAMET and considerable investments, co-funded by the European Union and the national metrology institutes, this research collaboration has reached a degree of maturity that allows to take a further step into sustainable joint activities and services on a European level. These could be a joint strategic research agenda of the NMIs, shared research Infrastructures, the exchange and training of researchers, but also a more systematic and comprehensive stakeholder involvement for the joined development of strategic priorities, joint dissemination structures or expert advice for regulators, industry and the general society alike.

EURAMET expects these activities to have the form of sustainable networks based on existing or newly build structures that suit the technical targets and the stakeholders in the metrological subject field. In late 2017, EURAMET initiated a call for proposals in search for ideas for such networks which triggered a huge response among the European NMIs and DIs. Finally, EURAMET approved six European Metrology Networks (EMNs) chosen from those ideas in May 2018. To foster the implementation of the EMNs with additional funding especially in their early stage of development, a dedicated EMPIR call "Support for Networks" was launched in January 2018. These EMPIR joint network projects (JNPs) were expected to explicitly establish and support a long-term ongoing dialogue between the metrology community and relevant stakeholders.

The proposals submitted to this EMPIR call were then evaluated in November 2018 via an external review panel and the three networks with a major input from the European community in metrology in chemistry were among the JNPs that now receive additional funding by EMPIR. These are the EMNs on energy gases, traceability in laboratory medicine and climate and ocean observation.

The EMN on energy gases aims at addressing metrological issues related to a sustainable and transparent supply of energy from conventional (natural gas, liquefied NG) and renewable energy sources such as biogas/biomethane and hydrogen. A main driver at the European level is, among others, the European Directive on renewable energy (2009/28/EC). There is also a high

importance of the transport and distribution of energy gases on a pan-European scale, setting requirements on harmonised approaches for the measurement of energy traded across Europe. Fundamental challenges, such as setting the physical and chemical specifications needed for renewable gases to enter the existing natural gas grid or quality and safety requirements for using hydrogen as fuel for long distance transportation shall be addressed.

In laboratory medicine, metrologically-based quality assessment (QA) of clinical laboratory testing for in vitro diagnostic devices is no longer optional but is compulsory to meet European regulations such as (EU) 2017/746. The EMN intends to establish a collaborative network for traceability in laboratory medicine involving metrology institutes, proficiency testing (PT) providers, clinicians, and regulators. It aims to respond to priorities for the provision of services jointly identified in close cooperation with the international stakeholders in medicine, for stakeholder research needs, and to develop new standards. The EMN intends to provide a long-term, sustainable coordination that comprehensively underpins a legally endorsed European QA infrastructure by providing consistent services to any European stakeholder.

The third EMN involving metrology in chemistry is addressing Earth's climate change. Trustable global data are needed that require decadal observations of the Earth system to extract the small signals from noisy backgrounds. The observables are complex and require the coordinated efforts of the worlds NMIs, to achieve laboratory quality uncertainties from space, deserts & oceans. The network aims to establish a forum to collect requirements on the metrological needs related to climate monitoring and mitigation and ocean observation. Jointly with stakeholders it intends to define research priorities, strategies and roadmaps and create a European focal point for the provision of metrological guidance and associated services for the climate and ocean observation.

Further details are given on the webpages of EURAMET

This joint and task specific approach of NMIs and stakeholders in Europe for addressing common tasks in metrology covering primary standards and dissemination procedures reaching the end user is a new and very customer-oriented approach to metrology in Europe. It also optimises the resources of the NMIs in Europe by providing joined and complementary services.

At the same time, this approach also reflects the values established by CITAC in the chemical sector right from the beginning, namely to foster collaboration between all organisations involved in chemical measurements with the aim to improve international comparability of such measurements.

The build-up phase of these network projects is expected to start in 2019. All these are, however, long-term goals of society and metrology alike and I wish everyone involved the courage and power that is needed to make this approach successful!

MESSAGE FROM THE CITAC SECRETARY

HOW TEST LABORATORIES DEAL WITH THE METROLOGICAL TRACEABILITY CONCEPT

Ricardo Bettencourt da Silva // University of Lisbon, Portugal

In my professional career as technical assessor and trainer of accredited test laboratories, member of national and international working groups, and participant in workshops, I had the opportunity to observe how most test accredited laboratories understand the metrological traceability concept.

My experience as professor at the University was not particularly useful in this aspect since most students have no professional experience in test laboratories. At the University we try to take all opportunities to teach basic or more advances concepts on metrology.

My description of how laboratories understand the metrological traceability concept is for sure biased by my specific experience in some analytical fields and by how I distribute my attention in the various aspects of the analytical work.

If it is asked an open question to a laboratory about the traceability of measurement results (requirement 5.6 or 6.5 of the previous and new ISO 17025 standard), most laboratories will present the calibration certificates of the balance, burette and/or the assessment of the temperature of the oven used in relevant operations of the test. Some of the laboratories would even present the calibration certificate of the thermometer used to check the preservation conditions of the sample (e.g. temperature of the freezer). Only few of them would add to this discussion the used reference materials of the chemical parameter. The accredited laboratories seem to be moderately careful in selecting the used reference material/standard for the chemical measurements by buying these to reputable institutions.

Occasionally, laboratories have problems attributable to the quality of the used chemical standard that becomes difficult to detect since most analysts are not aware of possible fragilities in calibrators values.

Fragilities in standards of inorganic analytes, such as metals or ionic species, are not frequent but the same cannot be said about some organic analytes, in particular for the most labile and difficult to purify.

When some years ago I worked in an accredited laboratory for the official monitoring of contaminants and residues in foodstuffs, I detected a difference of about 30% in the content of two lots of the same purified analyte provided by the same producer. This difference was detected because we had in place a procedure to compare every new lot of a reference substance with the previous one to check the quality and stability of the expensive reference substances in order to extend their shelf-life. The two reference substances are analysed

in their validity period after being preserved in the conditions defined by the producer. The new reference had and amount 30% less than the previous lot.

After some experimental checks of the difference, we moved our attention to the certificates of the reference substances. The purity of both reference substances was determined by the manufacturer by using the Total Area Method supported on different instrumental methods of analysis (GC-FID and GC-MS) that detect different impurities or the same impurities with different sensitivity. After reporting the finding to the provider, we got back apologies for the observed different in the contents.

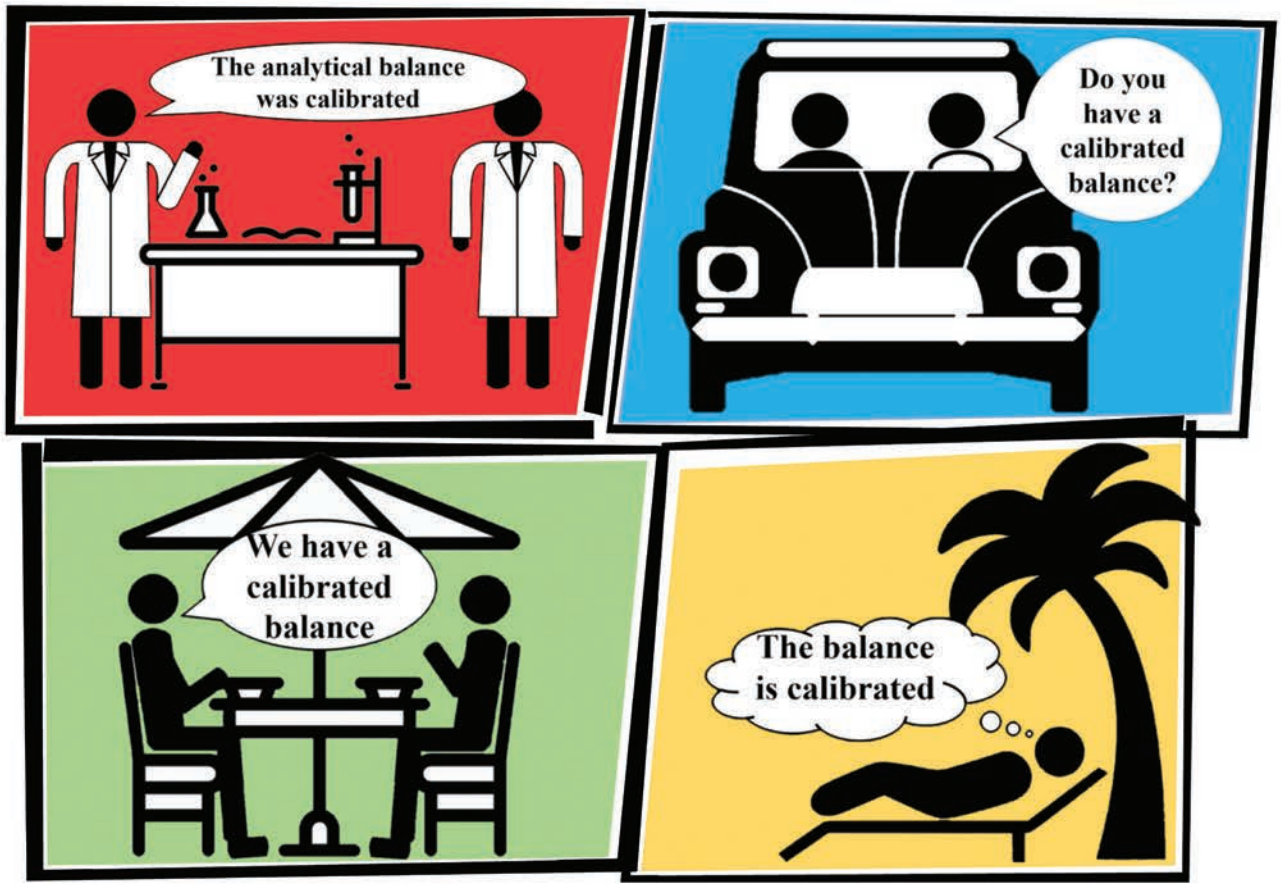
It is well known that the Total Area Method supported on GC-FID or GC-MS is not the most convenient way of determining the purity of purified chemicals, but not many analysts are fully aware of the problem or willing to pay more for reference substance of controlled quality.

Meanwhile, some analysts will justify their option for cheap references with the large dispersion of results from interlaboratory studies. However, in some cases this difference is also caused by differences in used references.

Some providers of purified reference substances are investing in qNMR determinations of the content of their products but this investment will only be successful if the community is aware of the possible impact of used references in the quality of their work.

CITAC is aware of this and of many other threats to the comparability of measurements in chemistry and will participate actively in promoting good practices.

The traceability of physical measurements performed in chemical tests is not enough to guarantee the adequate traceability of measurement results of chemical parameters.



EDITORIAL: THE CORRELATION BETWEEN US

Ilya Kuselman // Independent Consultant on Metrology, Israel, CITAC News Editor

A year after the preparation of the CITAC News 2018 has passed so quickly – time really speeds up with age. I understand now more the Rubáiyát of Omar Khayyám, where he suggests: "Be happy for this moment. This moment is your life"...

In the present issue you will find again messages of the CITAC officers, liaison reports, summaries of the CITAC Award winners, messages of the new members, reports from the events with the CITAC participation and announcements. There is also a new section "Changing the World of Metrology in Chemistry" containing information about the new mole in the new International System of Units (SI), creation of a new sister organization ForMEQ – The International Forum on Metrology and Examinology in Chemistry (of the Portuguese speaking countries), and the recently joining Ukraine to the Metre Convention. Another new section "Visit a CITAC member at his/her Lab" is a possibility to take a closer look at some laboratories/institutions active in metrology in chemistry. Everybody can find information on the Internet, but here we have the privilege to become directly familiar with the organization which is either led by a CITAC member or he/she is working in it.

The UN General Assembly has declared the year 2019 as the International Year of the Periodic Table of Chemical Elements (IYPT 2019). In this regard an article of our Russian CITAC members is dedicated to the 150 years celebration of the Periodic Table of D.I. Mendeleev, the first Russian metrologist in chemistry. The IUPAC 100th Anniversary is also celebrated in 2019. More about that is in the liaison report by Dr. Zoltan Mester, President of the IUPAC Analytical Chemistry Division. In addition, I am pleased to propose for your attention messages of the Editors of Pure and Applied Chemistry, the official IUPAC journal; of Chemistry International, the news magazine of IUPAC; and of Talanta, a peer-reviewed scientific journal in pure and applied analytical chemistry.

Thinking about the journals and preparation of a paper for publication, I would like to put in a good word for reviewers. Paper authors wish instinctively to receive a complement to their findings, instead of that in many cases – strict comments of the reviewers. What is voluntary and what is obligatory in the choice of a mathematical statistical method or a chemical analytical method? Each of them is based on its assumptions, has

drawbacks and advantages. Other aspects of a paper may be questionable, unclear or inaccurate expressions to be corrected: "lookers-on see more than the players". However, not always a reviewer is right, and the authors' answer should be equally respected by the Editor in the *peer* review process. It is nice if the reviewer comments are well-intentioned and passed to the authors in the reasonable term, set by the journal. In general, "that which does not kill us makes us stronger". As a rule, critical comments of a competent reviewer help to improve the paper, and quite often the contribution of the reviewer is significant not less than that of a co-author. Many thanks for this anonymous support.

The reviewers in the field of metrology in chemistry are mostly known members of CITAC, Eurachem, IUPAC Analytical Chemistry Division, ISO REMCO and other sister organizations. Part of these specialists are simultaneously members of several working groups (project teams) in these organizations, accumulating and disseminating corresponding knowledge. Sometimes a disbalance of personal ambitions and abilities may happen: both are important, the question is only their conformity, otherwise a conflict is possible.

People are like porcupines (or hedgehogs) in the known dilemma: they huddle together for warmth on a cold day, and prick one another with the quills.

Despite this dilemma, every scientist is with his/her talents, and we should be patient to learn from each other, to understand other parties in a dispute, to achieve a consensus, to win from the teamwork. Then, a correlation between members of a working group or a project team is positive and fruitful. Let's be in touch...

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LIAISON REPORTS 2018 OF THE SISTER INTERNATIONAL ORGANIZATIONS

AFRIMETS REPORT

Angelique Botha // NMI, South Africa

1. SUMMARY OF GENERAL ISSUES

The 12th Intra Africa Metrology System (AFRIMETS) General Assembly (GA) took place in Enugu, Nigeria, from 16-20 July 2018. The GA was preceded by five Technical Committee (TC) meetings. The General Assembly started with a session open to all interested parties from Nigeria, the region and other stakeholders. Representatives from the Governor of the State of Enugu, the African Union Commission, the Pan African Quality Infrastructure, the International Organisation for Legal Metrology (OIML/BIML), the International Bureau for Weights and Measures (BIPM) and the development partners UNIDO and the PTB (Germany) gave presentations. The GA were attended by several local industry representatives and over 60 metrology representatives from all sub-regions in Africa. The open GA concluded with presentations by the AFRIMETS Chair, the Sub-regional metrology organisations (CEMACMET, EAMET, MAGMET, NEWMET, SOAMET and SADCMET/MEL) and the Technical Committees.

The Closed GA for the members of AFRIMETS and main stakeholders was conducted on 20 July. The Directors gave feedback from their meeting where the main discussion topics were;

- the effect of the redefinition of the SI on Africa and how AFRIMETS should respond,
- the research projects in South Africa for a primary mass standard (Kibble/Watt balance and Avogadro sphere by 2020/21, supported by Kenya and Egypt),
- plans for a primary mass standard in Tunisia by 2030,
- how AFRIMETS should communicate the Revised SI to learners at schools and universities, and
- issues of reporting and financial sustainability.

The main recommendations from the Directors meeting were that the knowledge and information sharing in AFRIMETS should improve. The need for improved strategic planning was also discussed. There was a strong feeling that the organisation should move towards sustainability without external funding, i.e. that the implementation of a membership fee should be investigated. The Secretariat was tasked to present proposals on how membership fees and other income generation activities can be introduced at the next GA. The meeting also noted the need for a balance in activities between Scientific and Legal metrology and urged all structures of AFRIMETS to assist to ensure that Legal metrology activities are included in all activities of AFRIMETS.

Other issues that were discussed at the Closed GA were the AFRIMETS sustainability plan that was developed with the assistance of UNIDO and the introduction of an official course for a degree in metrology in the SOAMET region. The other sub-regions all gave updates on activities during the past year.

Other main resolutions of the Closed GA include:

1. Acceptance of South Sudan as the 46th member country of AFRIMETS,
2. Approval of the metrology institute of the United Arab Emirates as an Associate member of AFRIMETS,
3. Appreciation for NMISA (South Africa) for hosting the Secretariat for the past 11 years and for NRCS in support,
4. Noted the desire of Cameroon to host the GA 2020,
5. Encouraged the TC-QS to approve the QSs of institutes that want to submit CMCs.

The GA was viewed as successful with representation from most of the member countries covering all the sub-regions. A highlight of the GA was a visit to the building site of the new national metrology institute (NMI) of Nigeria. The first block of laboratories is completed, and the administration block and second block of laboratories are under construction.

The quality systems (QSs) of 8 national metrology institutes (NMIs) and two designated institutes (DIs) were presented to the AFRIMETS TC-QS. The meeting confirmed the approval of the quality systems of NSI (Namibia), ZMA (Zambia), SIRDC (Zimbabwe) and DEFNAT (Tunisia) as fit-for-purpose to support CMCs in the KCDB. The review of the QS of BOBS (Botswana) is still in progress.

The QSs of NMISA (South Africa), KEBS (Kenya) and NIS (Egypt) are up for the 5-year periodic review by the AFRIMETS TC-QS. NMISA and DEFNAT (Tunisia) will assist with KEBS and NIS, and NIS will assist with NMISA. The process for both NMISA and KEBS is expected to be completed by the end of 2018, since the two institutes are 3rd party accredited and this is in time for the expiry of the current approval (until early 2019). NIS would require an on-site visit to assess the non-accredited laboratories. This is planned for early 2019.

The migration of the AFRIMETS QSs to the new ISO/IEC 17025:2017 and ISO 17034:2016 standards was also discussed. A timeline has been agreed for all NMIs and DIs with CMCs to migrate to the new standards in the next 18 months. NMISA, KEBS, NIS, DEFNAT and the Associates are well on their way to migrate to the new

Fig. 1: Opening ceremony of the 12th Intra Africa Metrology System (AFRIMETS) General Assembly held in Enugu, Nigeria in July 2018

standards by the end of 2019. Ms Lerato Ntatamala, the Quality manager of NMISA, was elected to the TC-QS steering committee and will assist African NMIs/DIs to migrate to the updated standards.

2. CURRENT TC AND WORKING GROUP CHAIRS AND CONTACT DETAILS

The AFRIMETS structure includes working groups to mirror the international consultative committee working groups (CC-WGs) and are identified as TC-(parameter).

THE CONTACT DETAILS OF THE TC-CHAIRS IMPORTANT TO CHEMISTRY ARE LISTED BELOW:

Function	Name	Details
TC-QM Vice-Chair (Bio analysis)	Dr. Angelique Botha Mrs. Desirée Prevoo	National Metrology Institute of South Africa (NMISA), Private Bag X34, Lynnwood Ridge, 0040, RSA **Tel:** +27-12 8413800 **E-mail:** abotha@nmisa.org **Tel:** +27-12 8414576 **E-mail:** dprevoo@nmisa.org
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3. RMO MEMBERSHIP UPDATE

AFRIMETS has 6 sub-regional metrology organisations (SRMOs), which are primarily based on regional economic blocks, whose individual members are principal members of AFRIMETS. In total the SRMOs have forty two (42) members, thus AFRIMETS has 42 principal members. Countries not belonging to AFRIMETS through an SRMO are categorised as ordinary members. There are four (4) ordinary members, bringing the total number of members of AFRIMETS to forty-six (46).

The Associate members are the PTB (Germany), LNE (France), the NIRPR (National Institute of Radiation Protection and Research – Nigerian Nuclear Regulation Authority), GRPI (Ghana Radiation Protection Institute),

TAEC (the Tanzania Atomic Energy Commission), INSTN (Madagascar) and the International Atomic Energy Agency (IAEA). Observers include the European metrology organisation (EURAMET), the Arab Federation of Metrology (AFM), the African Committee of Metrology (CAFMET), the African Electrotechnical Standardisation Commission (AFSEC) and the Emirates Metrology Institute (EMI). Three institutes are designated by NMIs to participate in the Metre Convention on behalf of their governments:

South Africa: iThemba Laboratories for Medium and High-Energy Neutron Dosimetry

Tunisia: DEFNAT – Electricity
INRAP – Chemistry

Ethiopia (NMIE) and Tanzania (TBZ) became Associates of the International Conference of Weights and Measures (CGPM) in January 2018. The Members of the BIPM and Associates of the CGPM are shown below, as well as the participants in the CIPM MRA. Tanzania became the latest signatory to the CIPM MRA on 16 April 2018.

Member Country	Members of the BIPM	Associates of the CGPM	Signatories to CIPM MRA
Egypt	X		X
Kenya	X		X
Tunisia	X		X
South Africa	X		X
Botswana		X	X
Ethiopia		X	X
Ghana		X	X
Mauritius		X	X
Namibia		X	X
Seychelles		X	X
Sudan		X	X
Tanzania		X	X
Zambia		X	X
Zimbabwe		X	X

4. AFRIMETS CMCS

Zambia (ZMA) became the latest country in Africa to publish CMCs for the first time. As at 15 November 2018 there were a total of 634 CMCs accepted in Appendix C of the KCDB (General Physics = 473, Chemistry = 122 and IR = 39).

The CMCs originate from:

South Africa = 533 (118 CMCs in Chemistry)

Egypt = 39 (2 CMCs in Chemistry)

Kenya = 17 (2 CMCs in Chemistry)

Tunisia = 14

Zimbabwe = 13

Zambia = 11

Namibia = 7

It is expected that Ethiopia (NMIE), Botswana (BOBS) and Mauritius (MBS) will publish CMCs in the next year. Tunisia through INRAP is also expected to publish Chemistry CMCs soon as their quality system has been approved by the TC-QS.

5. DEVELOPMENT WORK IN CHEMISTRY

Most of the activities in Africa to improve the comparability of measurement results in the field of chemical and microbiological testing still focusses on standardisation. In Tanzania the Tanzania Bureau of Standards (TBS) performs testing over a diverse range of applications from microbiology, which is very important to ensure food safety, pharmaceuticals, cosmetics and forensic analysis. Tanzania also has more than ten testing laboratories that participate in the SADCMET Water proficiency testing (PT) scheme on an annual basis. In Ghana, the Ghana Bureau of Standards (GBS) also participates in the SADCMET Water PT and supports the mining industry. The Botswana Bureau of Standards (BOBS) and Kenya Bureau of Standards (KEBS) also performs testing to support food safety, water conservation, the mining industry and forensic analysis.

KEBS have established a capability in metrology in chemistry with an activity in gas analysis for the calibration of breath alcohol analysers and stack gas emission monitoring with a fourier-transform infrared (FTIR) spectroscopy measurement capability. In the field of food analysis KEBS has also started to publish CMCs and the institute also has an interest in a capability for the preparation of calibration standards for elemental analysis and a certified reference material (CRM) for maize, because it is very difficult to import the reference materials (RMs). INRAP, the designated institute for metrology in chemistry in Tunisia, has an interest in food safety specifically fish toxins and also experiences difficulties with the import of elemental calibration solutions and CRMs. INRAP is preparing to publish its first CMCs in the field of pesticides in fish in 2019 and is also developing a CRM.

The National Institute for Standards (NIS) in Egypt has established a capability for metrology in chemistry and started publishing CMCs in the field of cosmetics and organic solutions. Other countries that have an interest in establishing a new capability for metrology in chemistry in Africa including the Seychelles for medical gases and Ethiopia, are in the process of establishing its NMI.

The NMISA in South Africa has the most extensive capability for metrology in chemistry with laboratories for organic analysis that focusses on organic contaminants, such as persistent organic pollutants (POPs) and pesticides in food and environmental samples. The laboratory also has an advanced capability for purity assessment of high purity organic materials and most recently established a reference material production facility. The facility will focus on the preparation of CRMs relevant to food matrices found in Africa and is currently preparing for the certification of mycotoxins in a range of matrices such as white maize, as well as ground and tree nuts in collaboration with the national metrology institute (NIM) in China and the International Bureau of Weights and Measures (BIPM). The other laboratories include the Gas Analysis Laboratory that provides binary and multi-component primary reference gas mixtures (PRGMs) for a wide range of air pollutants including volatile organic compounds. The Inorganic Analysis Laboratory is also preparing to produce CRMs for toxic and nutritional elements in food matrices.

The NMISA held its inaugural Africa Food Safety Workshop from 4-8 June 2018 at The Capital Menlyn Maine in Pretoria, South Africa. The aim of the workshop was to share ideas, receive training and define a strategy on how the African region can ensure internationally acceptable monitoring and testing of food and feed, to protect the consumer against unsafe food products and to safeguard exports. The objectives achieved included mechanisms to improve food safety control systems on the African continent, while establishing and strengthening networks amongst food safety stakeholders.

The workshop brought together global representatives and delegates within the analytical regulatory food testing laboratories and metrology institutes, researchers in academia, governmental and non-governmental food programmes. The event also incorporated presentations and discussions with international experts on standards and methods of analysis and control for mycotoxins, veterinary drugs, pesticide residues and associated contaminants, including food traceability and authenticity with linkages to food microbiology, antimicrobial use and resistance. The NMISA has been

Fig. 2: ***Participants of the inaugural Africa Food Safety Workshop held in Pretoria, South Africa in June 2018***

selected to also host the second Africa Food Safety Workshop to be held in 2020.

6. FUTURE ACTIVITIES

The General Assembly 2019 will be hosted by NIS, Egypt in Cairo (8 to 12 July). Workshops on the implementation of the Revised SI and the harmonisation of analytical methods at the regional level are planned. APMP is invited to attend the workshops and GA. The AFRIMETS Secretariat plans to liaise with the APMP Secretariat on the APMP membership fee model as a possible model for AFRIMETS.

7. CONCLUSION

All AFRIMETS structures including the technical and quality system working groups are functioning well. Key and Supplementary comparisons are being conducted and it is expected that several new CMCs will be submitted by Associates during the next 1 to 2 years.

For any further information on the activities in AFRIMETS or the activities of the TC-QM for Chemistry, please contact:

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wlouw@nmisa.org
TC-QM Chair; Dr Angelique Botha
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TC-QM Vice-Chair; Ms Desirée Prevoo-Franszen
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APMP LIAISON REPORT

Tong Kooi Lee // Health Sciences Authority, Singapore

MID-YEAR MEETINGS

The Standards and Calibration Laboratory (SCL), together with the Government Laboratory (GL), hosted the 2018 APMP Mid-Year meetings and the "Metrology - Enabling Developing Economies in Asia" (MEDEA) Workshop from 3 to 6 July 2018 in Hong Kong. The mid-year meetings of the governance committees reviewed APMP's strategic directions, priorities and workplans, and included meetings of the Executive Committee (EC) members, Technical Committee (TC) Chairs, Focus Group Chairs and the Developing Economies Committee (DEC) members.

GENERAL ASSEMBLY AND RELATED MEETINGS

The A*STAR National Metrology Centre (NMC) and the Health Sciences Authority (HSA) jointly hosted the 34th APMP General Assembly and Related Meetings (APMP 2018) from 20 to 30 November 2018 in Singapore.

The event comprised the General Assembly (GA), meetings of the EC, TCs and the DEC, as well as satellite meetings, workshops for the TCs and the Focus Groups. A symposium was also organised as part of the activities of APMP 2018. Over 400 delegates/invited speakers from 30 economies attended the annual event.

APMP SYMPOSIUM "FUTURE OF METROLOGY – FUTURE OF INDUSTRY"

At the 26th meeting of the General Conference on Weights and Measures (CGPM) in Versailles, France, representatives of the International Bureau of Weights and Measures (BIPM)'s Members States unanimously voted for the redefinition of the International System of Units (SI) based on the fundamental constants. As APMP 2018 came after this historic decision, a symposium themed "Future of Metrology - Future of Industry" was organised. It provided a platform to share insights on the redefinition of the SI and its implications for the future of metrology and industry. Two breakout sessions, Track 1: SI Redefinition and its Impacts and Track 2: Metrology for Manufacturing and Digitalisation, were also organised.

The symposium included the following keynote addresses:

1. Dr Martin Milton, Director, BIPM: "The Redefinition of the Based Units of the SI: How We Achieved it";
2. Dr Terry Quinn, Emeritus Director, BIPM: "From Artefacts to Atoms"; and
3. Dr Takashi Usuda, Director, National Metrology Institute of Japan (NMIJ) and member of the International Committee for Weights and Measures (CIPM): "Redefinition of the SI – Strategy for National Metrology Institutes and the Industry".

APMP AWARDS

Dr Jia-Ruey Duann [Industrial Technology Research Institute (ITRI), Chinese Taipei] and Prof Prayoon Shiowattana [National Institute of Metrology Thailand (NIMT), Thailand) received the APMP and the APMP Developing Economy Awards for their contributions to APMP, respectively.

Dr Katsuhiro Shirono (NMIJ, Japan) received the 2018 APMP Iizuka Young Metrologist Prize while Dr Jariya Buajarern (NIMT, Thailand) received the Iizuka Young Metrologist Prize for Developing Economies.

Dr Huang Yu-Chung [Center for Measurement Standards (CMS)/ITRI, Chinese Taipei], Dr Murray Early [Measurement Standards Laboratory (MSL), New Zealand], Dr Lee Shih Mean (NMC, Singapore), Dr Tatsuya Zama (NMIJ, Japan), Prof Ma Liandi [National Institute of Metrology (NIM), China], Dr Isao Kishimoto (NMIJ, Japan), Dr Wang Li (NMC, Singapore), and Prof Prayoon Shiowattana (NIMT, Thailand) received the APMP Technical Activity Awards for having served their terms as TC Chairs and DEC Chair, respectively.

CHANGES IN EC & CHAIRMANSHIP OF TCS

Dr Osman Zakaria [National Metrology Institute of Malaysia (NMIM), Malaysia] and Dr Yu-Ping Lan (CMS/ITRI,

Chinese Taipei)'s terms as EC members were extended by one year. Ms Ajchara Charoensook (NIMT, Thailand) was approved as the new EC member. Mr Fang Xiang (NIM, China) was approved as the new APMP Chairperson. The new Chairs of other TCs were also approved.

METROLOGY - ENABLING DEVELOPING ECONOMIES IN ASIA (MEDEA)

MEDEA is a programme initiated under the APMP-Physikalisch-Technische Bundesanstalt (PTB) MoU with the aim of strengthening the development of metrology in the developing economies of the region. The programme implements its projects through the networks of APMP and APLMF (Asia-Pacific Legal Metrology Forum).

The second phase of the programme (MEDEA 2.0) takes place between 2018 and 2021. The training will include workshops, attachment and regional projects based on common interest.

ACTIVITIES OF THE TECHNICAL COMMITTEE FOR AMOUNT OF SUBSTANCE (TCQM)

The meeting was participated by 60 participants from 18 economies.

COMPARISONS

Since 1999, the APMP TCQM has organised 13 key comparisons (in the areas of gas and pH), 19 supplementary comparisons (in the area of gas and food), and 36 pilot studies (in the areas of food and biological materials, pH, water, cosmetics, inorganic solutions and surface). In line with APMP's Focus Groups' priorities on food safety, climate change and clean air, and clean water, the TCQM has organised a number of comparisons and proposed new ones to support the capability building efforts.

The recent APMP supplementary comparisons on *Elements in food supplement* and *Organochlorine pesticides in ginseng root* organised by GL, Hong Kong support the activities on "Metrology in Food Safety". The APMP pilot study on *Methane in nitrogen* organised by Korea Research Institute of Standards and Science (KRISS), Korea supports the activities on "Metrology in Climate Change and Clean Air". The pilot study on *Trace element in river water* organised by NMIJ, Japan aims to support the activities on "Metrology in Clean Water".

New proposed studies are underway as part of TCQM's efforts to support the activities of the Focus Groups. These include *Fipronil metabolite in chicken egg powder, Zearalenone in maize* and *anions in seawater* proposed by NIM, China, *Inorganic arsenic and elements in seafood* proposed by GL, Hong Kong and *Elements in lipstick material* proposed by HSA, Singapore.

Prior to the TCQM meeting, a two-day workshop on the topic of "Measurement and Capability Building in Residues of Veterinary Drugs in Meat & Seafood" and one-day workshop on the topic of "The Metrology Requirements for Clean Water" were organised. These workshops included technical presentations and discussions on issues related to capability building, training requirement and measurement traceability in greater depth.

CALIBRATION AND MEASUREMENT CAPABILITIES (CMCS)

As of 15 October 2018, a total of 2,394 CMCs from APMP in the QM area are published in the BIPM Key Comparison Database (KCDB). China, Korea and Japan are the three major contributors, having 886, 618 and 550 CMCs, respectively. Food (67.3%) and high purity chemicals (62.5%) are the two major contributors of APMP in the KCDB.

In Cycle XIX, a total of 253 new, revised or re-reviewed CMCs were submitted by eight economies from APMP, of which 226 were published on fast track.

FOCUS GROUPS

The five APMP Focus Groups cover issues that are priorities at the national and regional levels. This has led to a series of activities covering workshops and interactions with stakeholders:

- Climate change and clean air [chaired by Dr Sangil Lee (KRISS, Korea)]
- Food safety [chaired by Dr Hongmei Li (NIM, China)]
- Energy efficiency [chaired by Ms Ajchara Charoensook (NIMT, Thailand)]
- Medical metrology [chaired by Sheng-Jui Chen (CMS-ITRI, Chinese Taipei)]
- Clean water [chaired by Dr Ghufron Zaid (RCM LIPI, Indonesia)]

APMP-APLAC COOPERATION

The 5th APMP-APLAC Joint PT WG Meeting was held on 25 November 2018 as part of the activities of APMP 2018. The Joint PTs are planned to enhance the technical competence of field analytical laboratories in the Asia-Pacific region with metrologically traceable reference values provided by National Metrology Institutes/Designated Institutes (NMIs/DIs) for performance evaluation. To date, six PT schemes were completed. The following four PT schemes are being discussed and finalised:

- APLAC T106 (in parallel with APMP.QM-S11) Organochlorine pesticides (a-BHC & lindane) in ginseng root (GL, Hong Kong)
- APLAC T107 (in parallel with APMP.QM-S10) Elements (zinc, manganese, calcium & magnesium) in food supplement (GL, Hong Kong)
- APLAC T108 (in parallel with CCQM-K146) Benzo[a] pyrene in olive oil (NIM, China)
- APLAC T109 Cadmium in milk powder (NIM, China)

A new APLAC PT scheme on toxic metals/metalloid species (Cd, total As and inorganic As) in powdered rice has been formally submitted to APLAC in 2018 for approval.

UPCOMING MEETINGS

The 2019 Mid-Year meetings will be hosted by the Industrial Technology Development Institute (ITDI) in Cebu, Philippines. The 2019 GA and Related Meetings will be hosted by the National Measurement Institute, Australia (NMIA) in Sydney, Australia.

Delegates to the 34th APMP General Assembly

REPORT OF CCQM

Paola Fisicaro // Vice-chair of the Inorganic Analyses Working Group of the CCQM

The 24th CCQM meeting was held at BIPM, Sevres, in April 2018. The current organizational structure of the CCQM is based on eleven permanent working groups and one current ad hoc group. All the working groups had separate meetings with a growing numbers of participants.

Some of the main topics that have been discussed are summarized here. More detailed information is available (https://www.bipm.org/utils/common/pdf/CC/CCQM/CCQM24.pdf).

Dr May began the plenary meeting by providing a brief history of CCQM and the general objectives:

- Document and improve the world-wide comparability of measurements and measurement standards
- Improve chemical and biological measurement science
- Provide chemistry and biology metrology-related solutions to address important global/societal issues

The CCQM meeting has been the occasion to revise the strategic planning document for the 2017-2026, that was published on 18 January 2018. Dr Wielgosz showed how the document had been amended to fit the three objectives established for Consultative Committees by the CIPM, i.e. to progress the state of the art of measurement science, to reach out to new and established stakeholders, and to demonstrate the global comparability of measurements. The strategy document describes the CCQM's efforts to rationalise the comparison and CMC process, and details the strategies developed by the various working groups to develop core comparison models, which would allow a limited set of comparisons to support a broad range of CMC claims. Moreover, the document shows some case studies developed by CCQM WGs to provide good examples on the impact and long-term outcomes of selected key comparisons in the sectors of health care, environment, food safety, energy, advanced materials, and fundamental metrology and the SI (https://www.bipm.org/utils/en/pdf/CCQM-strategy-document.pdf).

During his update on the CIPM MRA review, Mr Henson noted that the CCQM has no significant gaps in addressing major recommendations from the CIPM MRA ad Hoc WG on Implementation. In addition, the CCQM's most recent strategic plan already reflects new objectives defined by the CIPM for the CCs. Mr Henson commented that the broad scope claims are one of the most complex issues facing the CIPM MRA review, in trying to decide what is covered and striking the right balance.

The progress of the task group on isotope ratio measurements and standards has been presented. Dr Mester reviewed the task group's activities, with an initial meeting in October 2017 held at VSL in Delft, Netherlands, and a second meeting held in April at BIPM that with a large number of participants. The mandate of the task group was to study the metrological state of isotope ratio measurements and formulate recommendations to the CCQM regarding potential engagement in this field. So far, several NMIs/DIs have activities in this field but these are spread out across different WGs. The creation of dedicated group not just focusing on compatibility but advancing isotope measurement science was recommended.

The CIPM approved the proposal of the CCQM to establish a CCQM Working Group on Isotope Ratio Measurement in June 2018.

Prof. Güttler, chair of the *ad hoc* working group on the mole, presented the progress of the group and the new definition of the 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 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."

It was noted that this new wording, where the unit is defined first followed by the definition of quantity, aligning the historical definition, will be easily accepted in the community and could be a good bridge between the redefinition of the mole and the teaching of chemistry.

Reports on the activities of the WGs and the RMOs were given by the respective chairs.

The CCQM is organizing a workshop for the celebrations of the 25th anniversary.

The workshop, entitled "Progressing the state of the art for Chemical and Biological Measurement Science", will be held on 10 April 2019. An associated poster session is planned for the evening of 9 April.

The 24th CCQM meeting in 2018 at the BIPM in Sèvres, France

REPORT OF COOMET TC 1.12 "REFERENCE MATERIALS"

S. Medvedevskikh // Chairman of COOMET TC 1.12 "Reference Materials"
O. Kremleva // Deputy Chairman of COOMET TC 1.12 "Reference Materials"
O. Anfilatova // The Coordinator

GENERAL

Activities on RMs in the framework of Euro-Asian Cooperation of National Metrology Institutions (COOMET) are carried out by Technical Committee 1.12 "Reference materials" (TC 1.12). The Committee includes representatives (Contact Persons) of 18 NMIs of the COOMET member countries: Armenia, Azerbaijan, Belarus, Bulgaria, Cuba, DPRK, Germany, Georgia, Kazakhstan, Kyrgyzstan, Lithuania, Moldova, Russia, Romania, Slovakia, Tajikistan, Ukraine, and Uzbekistan.

Dr. S. Medvedevskikh, Director of Ural Research Institute for Metrology (UNIIM), Russia, is the Chairman of TC 1.12.

In 2018 the work within TC 1.12 was carried out according to 24 registered COOMET projects, 3 of which were finalized**.** The Project Coordinators are experts from Russia and Ukraine. The experts from Belarus, Bulgaria, Kazakhstan, Kyrgyzstan, Moldova, Lithuania, Russia, Turkey, Ukraine and Uzbekistan participate in certification of CRMs developed according to the projects.

DEVELOPMENT OF COOMET CRMS

Cooperation within TC 1.12 is mostly aimed at the development and production of COOMET CRMs, which are permitted for use by national metrological bodies of COOMET member-countries without any additional research in their countries. This possibility is reached by participation in the required experimental work of the laboratories of the COOMET member-countries.

In 2018 such work was performed for 20 projects, including 3 new projects on CRM development:

729/RU/17 "Development of CRM of composition (agrochemical parameters) of brown heavy-loamy alkali soil SASolP-05";

732/RU/17 "Development of CRM set of refined gold composition";

733/RU/17 "Development of CRM set of refined platinum composition".

INFORMATION ON FINALIZED PROJECTS ON COOMET CRMS

The CRM of mass fractions of metals in slag of copper smelting production, developed by project **648/RU/14** "Development of CRM of mass fraction of metals in slag of copper smelting production" (the Project Coordinator - UNIIM, Ekaterinburg, Russia), was approved as the COOMET CRM at the 28th COOMET Committee meeting (April, 2018) and included in the Register of COOMET CRMs under the number **COOMET CRM 0114-2018-RU**. Armenia, Belarus, Bulgaria, Slovakia and Uzbekistan joined the recognition of the COOMET CRM.

The developed CRM of mass fractions of metals in slag of copper smelting production is intended for certification of measurement procedures, accuracy control of measurement results in the determination of a slag chemical composition, verification of metrological and technical characteristics of measurement instruments for conformity assessment of these instruments and their calibration procedures, and also for control of metrological characteristics of test results. Area of application: metallurgy, chemical industry, building industry, and scientific research.

The work on the project **732/RU/17** "Development of CRM set of refined gold composition" was also completed in 2018 (the Project Coordinator is OJSC "Krastsvetmet", Krasnoyarsk, Russia). Kazakhstan, Russia and Switzerland participated in this work.

At the 28th COOMET Committee meeting (April 2018)

the CRM for composition of refined gold was approved as the COOMET CRM and included in the Register of COOMET CRMs under the number **COOMET CRM 0115-2018-RU**. Belarus, Bulgaria, Kazakhstan, Kyrgyzstan and Slovakia joined the recognition of the COOMET CRM. The developed CRM is intended for calibration of measurement instruments, control of measurement results' accuracy and certification of measurement procedures, used for determination of composition of refined gold.

ORGANIZATION, COORDINATION AND METHODOLOGICAL SUPPORT OF ACTIVITIES FOR DEVELOPMENT OF CRMS IN THE FRAMEWORK OF COOMET

The annual updating of the Program of joint CRM development and production within COOMET (the on-going project **186/RU/99**) was completed, based on the analysis of the Program implementation in 2017-2018 and in view of the proposals, received at the 22nd and 23rd meetings of TC 1.12; decisions, taken at the 16th JCMS meeting and the 28th COOMET Committee meeting; proposals, submitted by the Contact Persons of TC 1.12 and RM producers of Russia. As a result of the updating, amendments were made to the Program concerning the information on the participants of certification analyses, the target dates for the work, new projects.

Assistance was provided to Project Coordinators in the preparation and submission of progress reports to TC 1.12 Secretariat, concerning the work on the projects, adjusting the stated deadlines in the work, etc.

The Secretariat of TC 1.12 updated the Register of the COOMET CRMs taking into consideration the decisions of the 28th COOMET Committee meeting to include 2 types of national CRMs of Russia in the Register of COOMET CRMs, to delete 4 types of CRMs of Bulgaria, and the information on the use extension of the national CRM certificates. The Register of the COOMET CRMs currently holds the information on 115 CRM types.

DEVELOPMENT OF NORMATIVE DOCUMENTS ON CRMS IN THE FRAMEWORK OF THE COOMET

In the period under review the Secretariat of TC 1.12 coordinated the work on the following projects.

697/RU/16 "Revision of COOMET Recommendation R/RM/22:2013 "Form and content of the COOMET certificate for reference materials of composition and properties of substances and materials". The question of revising COOMET Recommendation R/RM/22: 2013 was considered at the 23rd TC 1.12 meeting. As a result of the discussion at the meeting, it was decided to finalize the 2nd draft recommendation, agree it by correspondence in accordance with the established COOMET procedure and submit for adoption at the next COOMET Committee meeting.

543/AM/11 "Development and maintaining of the COOMET CRM Data Base (DB)". The information on the progress of the project was considered at the 23rd TC 1.12 meeting. Special attention was paid to the issue of the data generation and submission to the COOMET CRM Database using the prescribed form (structure) for the COOMET CRM Database in accordance with COOMET Recommendation R/RM/30: 2016. The decision was taken to request the Contact Persons of TC 1.12 to submit their comments and proposals to TC 1.12 Secretariat, concerning the preparation of the forms for national CRMs, recognized as the COOMET CRMs, accordingly to request of the Secretariat of TC 1.12 and the COOMET website administrator to update COOMET CRM DB in view of the obtained proposals.

The work on updating the page of TC 1.12 in the COOMET website **http://www.coomet.net/** was carried out.

COOPERATION WITH INTERNATIONAL AND REGIONAL ORGANIZATIONS

To coordinate the issues on RMs to be discussed in the framework of the COOMET, the liaisons with the leading international organizations in the field, such as ISO/REMCO, OIML TC 3/SC 3, CIS Interstate Council (NTCMetr), and the database COMAR, are regularly maintained. The Contact Persons of TC 1.12 participate in international meetings, representing the necessary information on the COOMET activities at these organizations. The information on participation of TC 1.12 members in international events on metrology in 2017-2018 was submitted to COOMET Secretariat for preparation of working papers for the 28th COOMET Committee meeting.

The articles, highlighting cooperation within COOMET and the information, covering RM activity in the framework of other international organizations: ISO/REMCO, BIPM, OIML, CIS Interstate Council (NTCMetr), and the database COMAR, are regularly published in "Reference Materials" journal, Russia.

INFORMATION ON THE 23RD TC 1.12 MEETING (SEPTEMBER 2018)

The 23rd TC 1.12 meeting was held on 14-15 September 2018 at UNIIM, Ekaterinburg, Russia. The meeting was attended by the representatives of 6 COOMET member-countries: Belarus, Germany, Kazakhstan, Russia, Ukraine and Uzbekistan, the representatives of TC 1.8 "Physical Chemistry", the experts in the RM area from leading metrological institutes of Russia – VNIIM and VNIIFTRI, and COOMET Project Coordinators from various branches of national economy of Russia, participating in the development of different types of COOMET RMs materials.

The agenda of the 23rd TC 1.12 meeting included traditionally RM activities, performed by national bodies of the countries, in the framework of ISO/REMCO and other international organizations; information of the Secretariat of TC 1.12 on the progress of the current projects of cooperation, concerning the development of COOMET CRMs and normative documents; on the progress of the Register and DB of COOMET CRMs, and maintaining the page of TC 1.12 at the COOMET website.

At the meeting, the Program of joint CRM production within COOMET (project **186/RU/99**), materials on the newly proposed projects on the development of COOMET CRMs, the question of drafting the form for updating COOMET CRM DB at the COOMET website (project **543/RU/11**) were considered. The decisions were taken on each issue under consideration, defining further action plan and target dates. The Minutes of the meeting TC 1.12 No. 23-2018 were prepared and signed by the representatives of COOMET member-countries.

The next 24th meeting of TC 1.12 is scheduled in Minsk, Belarus. The final venue and time of the meeting will be confirmed later.

Participants of the 23rd COOMET TC1.12 meeting

EURACHEM 2018 SUMMARY

Steve Ellison // Laboratory of the Government Chemist, UK

LEADERSHIP CHANGES

The Eurachem Chair and Vice-chair serve for a two-year term, with the vice-chair taking over from the current chair and appointment of a new incoming vice-chair. The chair for 2016-18, David Milde, accordingly stepped down and 2018 accordingly saw Marina Patriarca (Istituto Superiore di Sanità, Italy) taking over for her two-year term as Eurachem Chair. At the same time, the General Assembly elected Vicki Barwick (LGC, UK) as the new Vice-Chair, and appointed Francesca Rolle (Istituto Nazionale di Ricerca Metrologica, in Italy), as the new Secretary. The new Chair said "The main challenge ahead will be to support analytical laboratories facing the transition to the revised ISO/IEC 17025, by continuing to promote open discussion of common problems and the development of informed and harmonised approaches to technical and policy issues."

RECENT GUIDES AND INFORMATION LEAFLETS

Eurachem publishes a range of important guidance documents, many in collaboration with CITAC. Although no new Guides were published in 2018, Eurachem has published several translations, including German and Turkish translations of the well-known "Fitness for Purpose of Analytical Methods", covering method validation, Czech and Farsi translations of the Eurachem/CITAC guide "Quality in analytical chemistry – a Guide to Accreditation" and a new Russian translation of "Quantifying Uncertainty in Analytical Measurement" .

A new Eurachem Information Leaflet was also published: "ISO/IEC 17025:2017 - A New Accreditation Standard" covers the principal changes in the accreditation Standard ISO/IEC 17025, released in December 2017. Four translations of this leaflet are already available at https://www.eurachem.org/index.php/publications/leaflets/iso-iec-17025-2017. Many other information leaflets and were also translated into additional languages during 2018; news further details can see News pages at https://www.eurachem.org/index.php/news/newsarts.

WORKSHOPS

Eurachem continued its practice of arranging technical workshops in 2018, holding a successful international workshop on "Data – Quality, Analysis and Integrity" in Ireland in conjunction with the Eurachem General Assembly in May. The workshop included a range of oral and poster presentations; all the available presentations and poster copies are, in line with Eurachem's policy of open communication, available on the Eurachem website.

In 2019, the main Eurachem workshop will be the international workshop "Validation of targeted and non-targeted methods of analysis", to be held in Tartu, Estonia in May 2018. The workshop's main topic is validation of analytical methods – both targeted and non-targeted, where the question is more general such as determination of *any* organic contaminant in a given matrix, and targeted, where the analyte is clearly defined in advance. Further details can be found on the Eurachem website (see the end of this article) and at the workshop website at https://eurachem2019.akki.ut.ee/.

It is also notable that 2019 sees Eurachem celebrating the 30th year since its initial formation, and the General Assembly in 2019, and the associated workshop will see some celebratory retrospective activities.

CURRENT WORK PROGRAMME – PRINCIPAL ACTIVITIES

Eurachem's work programme includes the development of guidance documents as well as series of workshops. Several guides are under revision or in preparation. The Eurachem guide to establishing metrological traceability in chemical measurement (one of many joint activities with with CITAC) has been revised and was circulated for general Assembly comment and approval in 2018; the response was positive and we currently expect to publish the revised version in early 2019. The revision

primarily amends the guide – first published in 2003 – to reflect revised terminology introduced in the third edition of the VIM. Other work related to metrological traceability included a perception survey, released in early 2019, to help Eurachem understand how analysts and other measurement scientists interpret metrological traceability; the survey (initially open for contributions via http://bit.ly/EUCHM_TRC_2019) will help to inform future Eurachem policy and guidance on this key topic.

The Eurachem/CITAC working group on measurement uncertainty and metrological traceability is also working towards new guidance on the use of validation data for evaluation of measurement uncertainty; this is intended to give more detail of data requirements for this purpose, and of the combination of information on recovery or bias, precision etc. to form a viable uncertainty statement.

In addition to maintaining its broad collection of information leaflets, the Eurachem PT working group is working on guidance on the evaluation of qualitative results in PT schemes. Qualitative schemes include, for example, schemes aimed at confirming species identity, including microbiological species; some types of haematology, and some forensic activities. An initial survey of current methodology and needs was conducted in 2018. The new guide will help laboratories understand different evaluation methods and should be of use to proficiency testing providers hoping to set up qualitative schemes.

The Education and Training working group has continued to maintain the comprehensive Eurachem reading list, which provides pointers to almost 300 books, guides, standards, information notes and papers about analytical quality, collated by topic. This year's update includes about 40 improvements. The group is also working on a revision of another well-known Eurachem Guide; "Terminology in Analytical Measurement: Introduction to VIM 3", first published in 2011. The update extends the guide and updates some parts in line with more recent literature on metrological terminology.

Eurachem's method validation working group is also active; although the Fitness for Purpose Guide is not yet due for review, the group initiated an enquiry for comments on the present version and invites further comments. Comments on the document can be provided via an online form; a link can be found on the working group web page or in the announcement at https://www.eurachem.org/index.php/news/newsarts/243-nws-ffp-fdbk.

Eurachem is also working on a revision of the guidance document 'Selection and Use of Reference Materials'. The document was developed in 2002 and a modest amendment published as ILAC G9. Although the new version of ISO REMCO Guide 33 provides substantially more guidance on selection and use of reference materials, Eurachem feels that there is still a need for shorter, freely accessible guidance for laboratories who find it difficult to justify the purchase of a complete ISO document. Eurachem is also, often, in a position to provide translations of guidance into Eurachem member languages. Revision of the present joint guidance will accordingly help a wider range of laboratories choose and use reference materials appropriately.

2018 also saw considerable activity from the Eurachem Sampling Uncertainty working group. The group is has been busy updating the joint Eurachem/CITAC guide "Measurement uncertainty arising from sampling"; the update will include improved methods of handling skewed data and on reporting sampling uncertainty when the uncertainy interval is appreciably asymmetric. The revised version will be issued for comment in early 2019.

Finally, the Eurachem qualitative analysis working group continues to work towards new guidance on the evaluation and expression of uncertainty in qualitative analysis. Although a discussion paper published in 2002 outlined some general principles, there remains a need for performance characterisation for qualitative test methods, and a perceived need for information on how confidence in the results can be quantified and communicated. The working group issued a consultation draft to clarify the need and, with a new chair appointed in 2017, is working to improve the consistency and completeness of draft examples before issuing a draft for comment.

COMMUNICATION

The Eurachem Website now sees approximately 1m raw hits annually, and is regularly updated to include new guidance, translations and information about forthcoming

events. The site was also includes features to make it easier to share content via social media. Eurachem also maintains active Twitter feeds: @EurachemEurope provides general news and announcements on website updates and relevant organisations, with particular attention to accreditation for analytical chemistry; @EurachemPT provides updates on the PT working group activity (including PT workshops) and @EurachemEvents provides general information about forthcoming events and an active feed during workshops.

Further news about Eurachem activities, as well as contact details and general information about Eurachem, can be found on the Eurachem website at https://www.eurachem.org/.

EURAMET REPORT

Michela Sega // INRIM, Italy

2018: A REVOLUTIONARY YEAR FOR METROLOGY

2018 was a fundamental year for metrology: the General Conference on Weights and Measures, held in November in Versailles, ratified a paradigm change in the world of metrology. The international community voted to redefine the International System of Units (SI) and the redefinition of the kilogram, the ampere, the kelvin and the mole implies that the new SI will be homogeneous and all the SI units will be linked to natural constants. This will ensure the future stability of the SI and open up new opportunities for the use of smart technologies. It is worthwhile to mention the very important contribution given by EURAMET to the SI revision, both with the work carried out within its Technical Committees and with the Joint Research Projects developed within the EURAMET's European Metrology Research Programs (EMRP and EMPIR). 43 Joint Research Projects have been focused on the broader scope of the SI so far, 10 of which gave a direct contribution to the SI redefinition, with the involvement of 39 National Metrology Institutes and Designated Institutes and researchers coming from academia, research institutes and industry.

2018 was also an important year towards the promotion of cooperation conceived in a broader scope within EURAMET. The EURAMET 12th General Assembly (GA), which took place in Bucharest, Romania from 28 May to 1 June 2018 hosted by INM, approved six proposals of networks to become the first set of European Metrology Networks (EMNs): Mathematics and Statistics, Laboratory Medicine, Quantum Technologies, Smart Energy Grids, Energy Gases, and Climate and Ocean Observation. The EMNs have the purpose of bringing together the metrology institutes and the stakeholder in the relevant fields, to cooperate and work together and create sustainable structures for future collaborations. The six EMNs will sign their Memoranda of Understanding in 2019. During the GA, EURAMET chairmanship was transferred to the new Chairperson: Beat Jeckelmann (METAS, Switzerland) handed over to Hans Arne Frøystein (JV, Norway). In addition, Erkki Ikonen (VTT, Finland) was re-elected as EURAMET Vice-Chairperson for EMPIR related matters for a second term until 2021. The EURAMET Vice-Chairpersonship for GA is still hold by Maria Luisa Rastello (INRIM, Italy). EURAMET 13th General Assembly will take place in Borås, Sweden from 21 to 24 May 2019. It will be hosted by RISE, the Swedish National Metrology Institute.

In 2018 a Memorandum of Understanding was signed by EURAMET and another Regional Metrology Organization, COOMET, the Euro-Asian Cooperation of National Metrology Institutions. These two RMOs have a long tradition of partnership and currently run many complementary functions and this recent signing emphasizes the importance of strengthen the harmonized and collaborative global metrological infrastructure.

The cooperation among metrology institutes, academia,

stakeholders, will be implemented in 2019 within the EMPIR programme framework, via the usual two stage process, on the following major topics: energy, environment, normative research, research potential and support for networks. Stage 1, opening on the 9 January, aims at offering stakeholders from any country the opportunity to influence the projects undertaken by the European Community by identifying potential research topics. The highest priority topics received at Stage 1 will provide the basis for Stage 2 which will open in June. In addition, a call for support for impact projects designed to increase impact of completed projects will be launched in July 2019.

For the next long-term EU budget 2021-2027, the European Commission (EC) is proposing 100 billion euro for research and innovation. In order to continue the successes of Horizon 2020, an ambitious new program, Horizon Europe, will keep the EU at the forefront of global research and innovation. EURAMET is in discussions with national ministries and the European Commission over a potential European Partnership in Metrology, to follow on from the European Metrology Research Programs EMRP and EMPIR.

Technical collaboration in EURAMET is organized within ten Technical Committees (TCs), focusing on specific areas which represent the forum for scientific and technical cooperation in the respective fields. In addition, two Committees deal with the overall topics Quality and Interdisciplinary Metrology. The TCs are responsible for the execution of the activities required by EURAMET as RMO for the fulfilment of the Mutual Recognition Arrangement of the International Committee of Weights and Measures (CIPM-MRA). One of the ten TCs is devoted to Metrology in Chemistry (Technical Committee for Metrology in Chemistry, TC-MC), which is concerned with primary methods and reference materials for chemical measurements and research in metrology to support different sectors in the amount of substance fields.

NEWS FROM EURAMET TECHNICAL COMMITTEE IN METROLOGY IN CHEMISTRY (TC-MC)

TC-MC is chaired by Hanspeter Andres (METAS, CH). His mandate will end in May 2019 and the new Chairperson, who was appointed at the last EURAMET General Assembly, will be Sophie Vaslin-Reimann (LNE, France). In TC-MC, 28 EURAMET member countries are represented.

The technical activities is carried out within the four technical Sub-committees dealing with gas analysis (SC-GA), bio and organic analysis (SC-BOA), inorganic analysis (SC-IA), electrochemical analysis (SC-EA). The conveners of the subcommittees are: Janneke van Wjik (VSL, NL) for SC-GA, John Warren (LGC, UK) for SC-OA, Rainer Stosch (PTB, DE) for SC-IA and Daniel Stoica (LNE, FR) for SC-EA. In addition, a strategy working group, chaired by the TC-Chair, is also active on the following tasks: advice to TC-Chair and subcommittee conveners, strategic planning of comparisons, support actions, coordination, and organization of workshops.

The TC-MC members are actively participating in the European Metrology Programs EMRP and EMPIR, being involved in the various targeted programs (Health, Environment, Energy, Industry, Normative, Research Potential), thus indicating the cross-disciplinary nature of the TC itself.

TC-MC MEETING IN 2019

The annual meeting of the TC-MC was held from 4th to 7th February 2019 in Brno (Czech Republic) and was hosted by CMI. The first day was reserved for the conveners' meeting and for a dedicated workshop for DIs without CMCs five years after designation. The goal of the workshop was to understand the needs of the concerned DIs and define together appropriate actions, by discussing in depth all needs and requirements.

The four technical subcommittees reconvened, as usual, ahead of the annual TC-MC plenary meeting on 4th February 2019. A review of new claims as well as the obligatory re-review of a range of existing claims were carried out under cycle XIX of the CMC claim period. Running and new projects and comparisons in the framework of EURAMET and EMPIR and also proposals for the upcoming EMPIR call were discussed in detail in all sub-committees.

The plenary meeting took place the 6th and 7th February 2019. Some highlights on EURAMET, BIPM/CIPM, CCQM

strategy and activities within its main working groups were given. The conveners of the subcommittees gave an overview of the activities of each subcommittee and of the main outcomes of the meetings carried out in the previous day. A session of the plenary meeting was dedicated to European Metrology Networks (EMNs). After a general introduction on EMNs, an overview on the following EMNs, already approved by the EURAMET GA, dealing with topics related to the amount of substance field, was given: EMN on Climate and Ocean Observation (coordinated by NPL), EMN on Energy Gases (coordinated by VSL), EMN on Laboratory Medicine (coordinated by PTB). The following potential future EMNs were also presented: EMN on Environment (LNE), EMN on Precision Medicine and Advanced Therapeutics (LGC), EMN on Food Safety (INRIM).

The next TC-MC meeting will be held in Bern (Switzerland), from 4th to 7th February 2020.

ILAC LABORATORY COMMITTEE REPORT

Steve Sidney // LC Chair

The ILAC Laboratory Committee (LC) membership comprises international, regional and national associations of laboratories and associations of laboratory practitioners. ILAC stakeholders who do not fall within the ambit of the above definition are invited to meetings as guests of the LC.

The LC acts as the bridge between the ILAC member Accreditation Bodies (AB's) and the laboratory community as well as between the laboratory community and ILAC. Thus LC members have a dual role to play, on the one hand they represent their organisation in ILAC and on the other hand they represent the interests of the LC on various ILAC committees. The LC is therefore considered a conduit for laboratory input into ILAC and for ILAC output to the wider laboratory community.

In the past the LC conducted a closed meeting, however over the past 3-5 years a number of AB's, especially those who have only recently joined the ILAC MRA, have found it beneficial to attend the LC Meetings especially during the meeting held at the ILAC GA. The LC has accommodated this request and due to the continued interest shown by the AB's the LC took a formal decision to have a 'Closed Session', typically to be held on the first day of their meeting until the first coffee break and then to allow the rest of the meeting to be 'Open'. During the meeting in Singapore the 'Closed' part of the LC Meeting took place on Sunday 29th Oct from 08h30 – 10h30. The rest of the meeting, both on Sat 28th and the balance of the 29th was 'open'.

The proviso is that all non-LC Members are considered observers, and that should it be necessary extended 'Closed' time will be provided. Over the past few years this has worked extremely well and the same format was used this year in Singapore.

The LC has representatives on the following ILAC committees, Executive, Joint Executive (with IAF), ARC, AIC & PTWG, MCC, AMC and the newly formed Inspection Committee (IC). Members actively contribute to the work of those committees. In addition, currently the Chair represents ILAC at the BIPM Joint Committee on Guides in Metrology WG1.

There exists a wealth of experience within the LC Members and every year LC Members play their role in helping the ILAC Committees to fulfil their mandates.

The LC meets twice a year, once during the ILAC GA Meeting towards the end of each year and once during the March/April time period, at the same time as all the other ILAC Committees meet. This arrangement has, over an extended period of time, proved to be most beneficial and is both cost effective and value adding for

LC members. During 2018 the interim meeting was held in Frankfurt as has been the case for the past few years.

This report represents the period since the annual GA meetings held in Vancouver in 2017 and since these meetings are now being arranged by an independent event organiser the LC would once again like to congratulate the organiser as well as the ILAC/IAF Secretariats for the efficient and supportive arrangements that are made which result in these meeting being extremely productive.

LC HIGHLIGHTS SINCE LAST GA MEETING

- The official term (two years) of the Chair and Vice Chair of the LC are in line with other ILAC Committees and LC Members were advised during the mid-term meeting that nominations would be sought for both and voted upon at the Singapore meeting. The current Chair, having served three 2 year terms, indicated that he would not be available for the next term. At the time of writing this report the following nominations had been received.
  - Chair - Mr Jeff Gust (NCSLI – USA)
  - Vice-Chair – Dr Álvaro Ribeiro (Eurolab – Europe) and Mr R Singh (AOIL – India)

  During the "Closed Session" in Singapore voting will take place for these positions and the new officers will assume their role in January 2019.
- Since the LC meeting in Frankfurt, the 'white paper' regarding issues surrounding accreditation harmonisation anomalies, was published by the LC and submitted to the Chair of ILAC. This has subsequently been distributed to all members with a view to having in-depth discussions regarding various issues that were highlighted in survey. Initially these will be between the ILAC Executive and the LC and it is hoped that some time can be found during the Singapore meetings for this to take place.

  In addition to the paper mentioned in the last bullet point, the most significant issue that was discussed during both the Vancouver meeting in 2017 and the Frankfurt meeting earlier this year, were the changes that are envisaged by the revision of the ILAC Articles of Association (AoA).
- The LC made two major comments when requested to provide inputs.
  - Virtually unanimously the LC supported the concept of one vote per member AB
  - Many LC Members were concerned regarding the fact that the stakeholder representation on the Executive wouldn't have a vote and that the significance of the Lab Stakeholders might be diminished in terms of the new structure. These concerns were communicated to the Chair and the Executive and whilst the final outcome of the proposed changes to the AoA have not yet been agreed, changes reflecting these concerns have been made. Further discussion will be held during the upcoming LC Meeting in order to obtain the LC members view as a result of these changes.

A presentation with updated information from the Singapore Meeting will be made at the ILAC GA Meeting.

IMEKO REPORT

Michela Sega // INRIM, Italy, IMEKO TC8 Chair

IMEKO, the International Measurement Confederation, founded in 1958, is a non-governmental federation of 41 Member Organizations individually concerned with the advancement of measurement technology. Its fundamental objectives are the promotion of international interchange of scientific and technical information in the field of measurement and instrumentation and the enhancement of international co-operation among scientists and engineers from research and industry. Its Secretariat is located in Budapest (Hungary) and the Secretary is Mrs. Judit Farago. More information about IMEKO and its structure can be found on the IMEKO

website (www.imeko.org).

In 2018, new IMEKO Officers and Chairs of IMEKO Committees were elected or re-elected for the next three-year mandate (2019-2021). In particular, Prof. Masatoshi Ishikawa (Japan) was elected as the new President of IMEKO. Prof. Frank Härtig (Germany) is the new President Elect and the Chair of the Technical Board.

The biggest IMEKO event in 2018 was the IMEKO XXII World Congress 2018 (www.imeko2018.org), held in Belfast (Northern Ireland, UK) from 3rd to 6th September 2018, which took place in the Belfast Waterfront Conference & Exhibition Centre. An effective and great organizational work was carried out by the Institute of Measurement & Control (Inst MC), the host UK Member Organization of IMEKO and the National Metrology Institute of UK, the National Physical Laboratory (NPL), supported by a Congress Organizing Team from a professional service provider. The Congress was a very successful one, with 581 participants from various Countries and 465 scientific presentations. It was organized in five plenary sessions and a number of parallel sessions. During the plenary sessions, notable key-note speakers gave fascinating lectures, including two Nobel Prize Laureates, Prof. William D Phillips (Nobel Prize in Physics in 1997) and Prof. Klaus von Klitzing (Nobel Prize in Physics in 1985), as well as the BIPM Director, Dr. Martin Milton. A big exhibition area with 21 UK industries was also visited by the attendees in the congress venue. The Congress had also an interesting social program, which included the visit and the social dinner at the spectacular Titanic Belfast.

The next XXIII IMEKO World Congress will be held in Yokohama (Japan) on 30 August -3 September 2021. It will be hosted by the Japanese Member Organization of IMEKO, the Society of Instrument and Control Engineers (SICE), with active involvement from many Japanese professional bodies, universities and industry. More information can be found in the website www.imeko2021.org.

In 2018, the IMEKO Online Journal ACTA IMEKO, published its 4 issues (https://acta.imeko.org/index.php/acta-imeko); the most recent one (Vol 7, No 4, Year 2018) appeared in December 2018.

REPORT FROM ISO/REMCO

Angelique Botha // National Metrology Institute of South Africa (NMISA), ISO/REMCO Chair

The 41st meeting of the Reference Material Committee of ISO, ISO/REMCO, was held in Ottawa, Canada from 10–13 July 2018, and was hosted by the National Research Council of Canada (NRCC). ISO/REMCO now has a membership of 71 members of the International Organization for Standardization (ISO), liaison with 16 international organizations and multiple ISO-internal committees (9 'to' and 24 'from' ISO/REMCO). Thirty-four delegates and liaison representatives attended the meeting coming from 12 ISO participating (P) members out of 32 (37%), 1 internal ISO technical committee in liaison out of 9 (11%) and 5 international organizations in liaison out of 16 (31%).

The scope of ISO/REMCO, as agreed by the ISO Technical Management Board (TMB), is:

- To establish concepts, terms and definitions related to reference materials;
- To specify the basic characteristics of reference materials as required by their intended use;
- To propose actions on reference materials required to support other ISO activities;
- To prepare guidelines for ISO technical committees when dealing with reference material issues;
- To communicate with other international organizations on reference material matters;
- To advise the ISO TMB on reference material issues.

MEMBERSHIP UPDATE AND LIAISON COORDINATION

The strong liaison relationships that ISO/REMCO has built up with international organisations, such as ISO/CASCO and ILAC over past years continues to be invaluable this year. With the publication of the new international standard for the competence of reference material producers (ISO 17034), and the latest revision of ISO/IEC 17025 the emphasis of ISO/REMCO is shifted to updating terminology. This activity coincides and is in collaboration with the current draft revision to the International Vocabulary of Metrology (VIM 4). Furthermore, ISO/REMCO is working towards providing additional specific guidance in new focused areas of reference material production and use; updates on which are detailed below.

As currently defined in ISO 17034 a certified reference material (CRM) is a reference material (RM), where in addition to the stated requirements for the RM, the metrological traceability of the certified value is stated, together with an estimate of the uncertainty of the property value. As discussed later, these clear additional requirements for a CRM relates to the '...one or more property values' that are certified, and not the physical reference material itself, which was one of the key discussion points in the session on 'Terminology'.

NEW OPPORTUNITIES FOR THE PROMOTION OF THE WORK OF ISO/REMCO

At the meeting, there was also a presentation of the ISO/REMCO website currently in development. This website resides within the overall ISO website, and follows ISO defined design and structure. However, these Technical Committee sites are defined to promote, and share news, information etc., together with the more structured ISO website. The development continues with the website made available in October 2018 at https://committee.iso.org/home/remco.

BRAINSTORMING SESSION ON THE COMMUTABILITY OF REFERENCE MATERIALS

From the discussions, the REMCO members gained a better understanding that commutability is an approach used by the clinical chemists to correct for biases between routine samples and reference materials (RMs) for different methodologies. In the analytical chemistry community this is usually described as matrix effects. The analytical chemist will usually work on the method to eliminate the biases as far as possible. In clinical chemistry the limited access to the intellectual property of the technologies often make it difficult to define the measurand in sufficient detail to be able to eliminate the biases.

Commutability therefore has a lot to do with the intended

Group photo taken at the 4st annual ISO/REMCO meeting held in Ottawa, Canada in July 2018

use of the material. In terms of reference materials, the requirement to assess the commutability of the material will be the responsibility of the reference material producers (RMP) as far as the intended use of the material stated on the RM document. If the user wants to use the material outside the stated use on the RM document, it will be the responsibility of the user to assess the commutability of the material for the intended use. Dr Steve Ellison who originally drafted the REMCO position paper on commutability was asked to update it for a 12-week committee internal ballot to be discussed for finalisation at the 42nd ISO/REMCO meeting in June 2019.

BRAINSTORMING SESSION ON TERMINOLOGY RELATED TO REFERENCE MATERIALS

During the brainstorming session on terminology a need was identified to review some of the REMCO definitions including the definitions for certified value, certified reference material (CRM), the period of validity of the RM document and the lifetime of a reference material. A need was also identified to review the different terms used by different RMPs for values reported on the CRM certificate that are not certified values, such as reference values, information values, etc. Now REMCO only has the one term - indicative values - to include all the values reported on the certificate that are not certified values. REMCO could also consider developing terminology for qualitative property values, including nominal and (discrete) ordinal properties. The discussions at the brainstorming session identified the need to reactivate working group (WG) 10 on the terms and definitions related to reference materials for the possible amendment of ISO Guide 30.

The need for the strong liaison relationship with BIPM JCGM working group (WG) 2 (responsible for the International Vocabulary for Metrology – the VIM [3]) was also reinforced during the brainstorming session. ISO/REMCO is very grateful for the time and effort made by Dr Chuck Ehrlich, the convenor of JCGM WG2 to attend the brainstorming session. The REMCO members made the proposal to provide the current ISO Guide 30 definitions of reference material and certified reference material to JCGM WG2 for input into the minimal change committee draft of the VIM4 that is due by the end of November 2018. Any amendments required to be made to the definitions could then be finalised during the commenting stage of the committee draft. This will allow for the formal review of the REMCO definitions through the ISO consensus building process through the new working group (WG10) being established in parallel to the drafting of the VIM 4.

ISO/REMCO also support the proposal by ISO/TC 12 to go back to the 8th edition of the SI brochure definition for "unit" so that "units" are "quantities" and not "values of quantities" or "quantity values".

GUIDANCE ON THE PRODUCTION OF QUALITATIVE REFERENCE MATERIALS AND THE ASSIGNMENT OF NOMINAL PROPERTIES

A new work item has been registered as ISO Guide 85 with the proposed title "Production of reference materials having one or more assigned qualitative property values". Stefanie Trapmann, the convenor of WG13, proposes to start the drafting of the working document with the structure that was originally proposed for the Guide before the Technical Report 79 was developed.

The development of the Guide will involve some discussions about terminology for qualitative properties, including nominal properties, ordinal properties or ordinal discrete property values, but a sincere attempt will be made not to make it the focus of the Guide. The contents of the Guide according to the proposed structure will be facilitated through updating the examples used in TR 79 and using examples proposed by experts who are already members of WG13 or who are willing to become members of WG13. The WG will exclude guidance on the use of qualitative RMs in the Guide but will collect the information on the use of qualitative RMs for inclusion in the next revision of ISO Guide 33. The plan is to discuss a working draft of the Guide at the 42nd meeting of ISO/REMCO.

GUIDANCE ON THE PRODUCTION OF HIGH PURITY REFERENCE MATERIALS

ISO Guide 86 has been registered as a new work item with the proposed title: Guidance on the production of high purity reference materials for small organic

molecules. A new working group (WG18) has been established under the convenorship of Dr Takeshi Saito. The membership of the new working group will consist of the existing members of the ad-hoc group 4 that looked at the possibility of developing guidance for high purity reference materials. A new ad-hoc group under the convenorship of Dr Zoltan Mester has been established to consider the development of guidance on the production of high purity inorganic reference materials. This group will prepare a new work item proposal for a 12-week committee internal ballot before the next ISO/REMCO meeting.

During the committee internal balloting for the new work item proposal for ISO Guide 86, some comments were received from the REMCO members. These included whether the scope will only cover pure natural organic molecules or also synthetic molecules, the Russian Federation has a state system document on purity reference materials, which is in the process of being translated into English and could provide relevant input to the REMCO guidance document. The UK made a strong recommendation that the REMCO guidance document should not duplicate the IUPAC project on high purity materials. During the initial discussions in ad-hoc group 4, it was already clarified that the guidance document will focus on reference material issues and that the IUPAC project will be included as a valuable reference in the Guide. Some comments were received from ISO/TC 158 (Gas analysis). The committee recently published an international standard on purity analysis for gases. Other scope questions included the definition of small organic molecule and that the focus of the document will be on quantitative analysis and not qualitative (identity).

The proposed outline for the Guide will follow the structure of ISO 17034 with general requirements for the production of high purity materials, structural resources from clauses 5 and 6, but the focus will be on the technical requirements. The topics that will be focussed on include the assessment of homogeneity, the assessment and monitoring of stability, metrological traceability, characterisation with specific reference to direct and indirect methods and the treatment of non-detected impurities when the indirect method is used, the combination of methods and the estimation of the uncertainty.

The 42nd meeting of ISO/REMCO will be held in South Korea from 9 to 13 June 2019.

REPORT FROM ISO/TC 69/SC 6

Tomoyuki Endo // ISO/TC 69/SC 6 Secretary

GENERAL

ISO/TC 69/SC 6 has Secretariat situated in Japan (JISC), 15 participating and 18 observing members. There are in liaison 13 ISO committees and 5 international organizations (European Commission, International Dairy Federation, International Olive Council, ILAC, IMEKO and OIML). The standards published by ISO/TC 69/SC 6 are listed in the following table.

Reference	Document title
ISO 5725-1:1994	Accuracy (trueness and precision) of measurement methods and results -- Part 1: General principles and definitions
ISO 5725-2:1994	Accuracy (trueness and precision) of measurement methods and results -- Part 2: Basic method for the determination of repeatability and reproducibility of a standard measurement method

Reference	Document title
ISO 5725-3:1994	Accuracy (trueness and precision) of measurement methods and results -- Part 3: Intermediate measures of the precision of a standard measurement method
ISO 5725-4:1994	Accuracy (trueness and precision) of measurement methods and results -- Part 4: Basic methods for the determination of the trueness of a standard measurement method
ISO 5725-5:1998	Accuracy (trueness and precision) of measurement methods and results -- Part 5: Alternative methods for the determination of the precision of a standard measurement method
ISO 5725-6:1994	Accuracy (trueness and precision) of measurement methods and results -- Part 6: Use in practice of accuracy values
ISO 10576-1:2003	Statistical methods -- Guidelines for the evaluation of conformity with specified requirements -- Part 1: General principles
ISO 10725:2000	Acceptance sampling plans and procedures for the inspection of bulk materials
ISO 11095:1996	Linear calibration using reference materials
ISO 11648-1:2003	Statistical aspects of sampling from bulk materials -- Part 1: General principles
ISO 11648-2:2001	Statistical aspects of sampling from bulk materials -- Part 2: Sampling of particulate materials
ISO 11843-1:1997	Capability of detection -- Part 1: Terms and definitions
ISO 11843-2:2000	Capability of detection -- Part 2: Methodology in the linear calibration case
ISO 11843-3:2003	Capability of detection -- Part 3: Methodology for determination of the critical value for the response variable when no calibration data are used
ISO 11843-4:2003	Capability of detection -- Part 4: Methodology for comparing the minimum detectable value with a given value
ISO 11843-5:2008	Capability of detection -- Part 5: Methodology in the linear and non-linear calibration cases
ISO 11843-5:2008/ Amd 1:2017	Capability of detection -- Part 5: Methodology in the linear and non-linear calibration cases -- Amendment 1
ISO 11843-6:2013	Capability of detection -- Part 6: Methodology for the determination of the critical value and the minimum detectable value in Poisson distributed measurements by normal approximations
ISO 11843-7:2012	Capability of detection -- Part 7: Methodology based on stochastic properties of instrumental noise
ISO 13528:2015	Statistical methods for use in proficiency testing by interlaboratory comparison
ISO 21748:2017	Guidance for the use of repeatability, reproducibility and trueness estimates in measurement uncertainty evaluation
ISO/TR 13587:2012	Three statistical approaches for the assessment and interpretation of measurement uncertainty
ISO/TR 22971:2005	Accuracy (trueness and precision) of measurement methods and results -- Practical guidance for the use of ISO 5725-2:1994 in designing, implementing and statistically analysing interlaboratory repeatability and reproducibility results

Reference	Document title
ISO/TS 17503:2015	Statistical methods of uncertainty evaluation -- Guidance on evaluation of uncertainty using two-factor crossed designs
ISO/TS 21749:2005	Measurement uncertainty for metrological applications -- Repeated measurements and nested experiments
ISO/TS 28037:2010	Determination and use of straight-line calibration functions

WORKING GROUPS

WG 1 „Accuracy of measurement methods and results": Prof. Ojima

Revision of ISO 5725 series

ISO/AWI 5725-1 *Accuracy (trueness and precision) of measurement methods and results -- Part 1: General principles and definitions.* The project leader: Ms. Soraya Amarouche.

ISO/TC 69/SC 6/WG 1 agreed to register this project as PWI stage to avoid an automatic cancellation and to initiate WG consultation to review a draft well before restarting this project. ISO/TC 69/SC 6/WG 1 requested the project leader to prepare a draft by 2018-07-06.

ISO/CD 5725-2 *Accuracy (trueness and precision) of measurement methods and results -- Part 2: Basic method for the determination of repeatability and reproducibility of a standard measurement method.* The project leader: Dr. Steve Ellison.

ISO/TC 69/SC 6/WG 1 requested the project leader to prepare a draft by 2018-8-15 for WG consultation and agreed to proceed to the DIS after the consultation.

ISO/NP 5725-3 *Accuracy (trueness and precision) of measurement methods and results – Part 3: Alternative designs for precision studies.* The project leader: Dr. Steffen Uhlig.

ISO/TC 69/SC 6/WG 1 agreed to initiate WG consultation to review a draft well. ISO/TC 69/SC 6/WG 1 requested the project leader to prepare a revised draft by 2018-10-31.

ISO/CD 5725-4 *Accuracy (trueness and precision) of measurement methods and results -- Part 4: Basic methods for the determination of the trueness of a standard measurement method.* The project leader: Prof. Jiang Zheng.

ISO/TC 69/SC 6/WG 1 requested the project leader to prepare a revised draft by 2018-7-06 for WG consultation and agreed to proceed to the DIS after the consultation.

ISO/PWI 5725-5 *Accuracy (trueness and precision) of measurement methods and results -- Part 5: Alternative methods for the determination of the precision of a standard measurement method.*

ISO/TC 69/SC 6/WG 1 agreed to start revision of part 5 after the current revision work part1, part2, part3, part4).

ISO/NP 27877 *Precision of binary data.*

ISO/TC 69/SC 6/WG 1 agreed to change the project leader, from Prof. Tomomichi Suzuki to Dr. Jun-ichi Takeshita.

ISO/NP 27878 *Reproducibility of the LOD of binary methods by means of collaborative studies.* The project leader: Dr. Steffen Uhlig.

ISO/TC 69/SC 6/WG 1 agreed to initiate WG consultation and requested the project leader to prepare a revised draft by 2018-11-30.

WG 5 „CAPABILITY OF DETECTION": DR. HAYASHI

Systematic review of ISO 11843-6:2008 (v. 2) *Capability of detection -- Part 5: Methodology in the linear and non-linear calibration case.*

ISO/TC 69/SC 6/WG 5 discussed the result of systematic review. Although a simple majority of voting P-members has proposed confirmation, Finland and Japan proposed revision/Amend with some comments. As result of discussion, they conduct minor revision to correct editorial issue.

New proposal of Guidance for the implementation of ISO 11843 series

Dr. Hayashi, the convener of ISO/TC 69/SC 6/WG 5, proposed to develop a document which makes the parts of ISO 11843 series easily understandable for users. ISO/

TC 69/SC 6 agreed to continue this item discussion and to register it as PWI with Dr. Hayashi as the project leader.

WG 7 "Statistical methods to support measurement uncertainty evaluation": Prof. Cox

ISO/NP TS 23471 *Experimental designs for evaluation of uncertainty – Use of factorial designs for determining uncertainty functions* .The project leader: Dr. Steffen Uhlig.

ISO/TC 69/SC 6/WG 7 agreed to conduct WG consultation. ISO/TC 69/SC 6/WG 1 requested the project leader to prepare a revised draft by 2018-11-30.

NEW PROPOSAL OF "THE EVALUATION OF THE UNCERTAINTY OF MEASUREMENTS FROM AN AUTOCORRELATED PROCESS"

Dr. Nien-fan Zhang presented document on "The evaluation of the uncertainty of measurements from an autocorrelated process". ISO/TC 69/SC 6/WG 7 agreed to initiate NP ballot to be registered as WD (stage 20.00). ISO/TC 69/SC 6/WG 7 requested the project leader to prepare a document for the NP by 2018-10-31. The secretary will arrange NP ballot with a 12 weeks' voting period.

MEETING ON ISO 13528: PROF. SUZUKI

Prof Suzuki, the chair of ISO/TC 69/SC 6, reported the outcome of meeting in Berlin 2018. The meeting agreed to call for comments on the structure and technical content of ISO 13528:2015 within committee members of ISO/TC 69/SC 6 by 2018-11-30. The meeting agreed to establish AHG with Prof. Tomomichi Suzuki as its convener.

IUPAC ANALYTICAL CHEMISTRY DIVISION REPORT

Zoltan Mester // National Research Council (NRC), Canada

IUPAC PROJECTS OF INTEREST

2013-048-1-100 Project on the redefinition of the mole, entitled: A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities has now been completed. IUPAC recommendation is available at Pure and Applied Chemistry 90 (1), pp. 175–180 (2018), https://doi.org/10.1515/pac-2017-0106. The new definition of the mole is: The mole, symbol mol, is the SI unit of amount of substance. One mole contains exactly 6.022 140 76×1023 elementary entities. This number is the fixed numerical value of the Avogadro constant, *NA*, 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.

2017-031-1-050 IUPAC100 Periodic Table Challenge .As a part of the 100 years of IUPAC and the 150 years of the Periodic Table, a sub project is preparing for The Global Periodic Table Competition. Division input would be appreciated in the form of potential questions. "Questions about the name, chemical or physical properties or discovery are possible. But more importantly, we also need you to provide the correct answer highlighting the role of IUPAC in that particular case or more broadly." This activity is about educating people about the work of IUPAC. In this context, we also note that the United Nations General Assembly has proclaimed 2019 as the "International Year of the Periodic Table of Chemical Elements". See IUPAC news 20th December 2017.

2012-005-1-500 Vocabulary of Concepts and Terms in Analytical Chemistry - the revised Orange Book project. The Orange Book (present title "Compendium of Analytical Nomenclature3 "rd Edition) was published in 1998, and now is in the process of revision. The new Orange Book will be in a consistent glossary style format with definitions of concepts in different fields of analytical chemistry. The nineteen chapters of the 3rd edition will become eleven in the present revision. We have taken

the decision to concentrate on methods and not attempt to venture into the ocean of applications. The first chapter will set the metrological scene with definitions from the Green Book, the International Vocabulary of Concepts and Associated Terms in Metrology (VIM) and selected chemometric and statistical terms. The project is nearing completing, publication is expected by the end of 2019.

2017-005-3-500 Analytical Chemistry of Nanomaterials. The impact of materials structured at the nanometer scale becomes enormous and continues to increase. Analytical chemistry of nanomaterials belongs to emerging issues in this field. Together with physical and physicochemical characterization of shape, size, and structure nanoparticles, analytical chemistry research considers isolation/purification and detection-identification/ quantification/ spatial composition characterization of nanomaterials in bulk materials, special nanotechnology products, complex matrices of environmental, biological and food samples, and others. The project intend to produce a guidance document on best analytical chemistry practices for the characterization of such materials.

2016-007-1-500 Risks of Conformity assessment of a multicomponent material or object in relation to measurement uncertainty of its test measurements. To develop an approach for evaluation of the probability of false decisions in conformity assessment of a multicomponent material or object in relation to measurement uncertainty of test (chemical analytical) results of a sample of the material or object. This probability, combining probabilities of false decisions concerning different components of the material or object, will characterize the sample conformity as a whole. The solution to this problem is important for understanding conformity assessment risks in customs control, clinical analysis, pharmaceutical industry, environmental control, and other fields.

2019 DOUBLE CELEBRATION

This year, IUPAC and world are celebrating the 150 years of the periodic table as outlined by Dmitri Mendeleev in 1869, and the 100 years since the founding of the International Union of Pure and Applied Chemistry (IUPAC). As stated in the prospectus of the International Year of the Periodic Table: 'In proclaiming an International Year focusing on the periodic table of chemical elements and its applications, the United Nations has recognised the importance of raising global awareness of how chemistry promotes sustainable development and provides solutions to global challenges in energy, education, agriculture and health' as proclaimed by the United Nations General Assembly and UNESCO. IUPAC along with International Union of Pure and Applied Physics (Iupap), the European Chemical Society (EuChemS), the International Science Council (ISC), International Astronomical Union (IAU), and the International Union of History and Philosophy of Science and Technology (IUHPS) spearheaded this effort celebrating chemical science and its contribution to development and betterment of life. The year opening at UNESCO in Paris, France on January 29th; its opening in Moscow, Russia on Mendeleev's birthday, February 8; the IUPAC100 global breakfasts on 12 February; and, following the International Day for Women and Girls in Science, the International Symposium on Women and the Periodic Table in Murcia, Spain, on February 11–12. Other major meetings through the year include the IUPAC Congress in Paris, which starts on 7 July, and Mendeleev 150, otherwise known as the 4th International Conference on the Periodic Table, in St Petersburg, Russia on July26–28, https://www.iypt2019.org/.

IUPAC100 PERIODIC TABLE OF YOUNGER CHEMISTS

Co-sponsored by the International Younger Chemists Network (IYCN). Contact Person: Christine Dunne, ptchemists@iupac.org

In celebration of the 100th anniversary of IUPAC and the International Year of the Periodic Table, IUPAC and IYCN announce the creation of a Periodic Table of Younger Chemists. Beginning in July 2018 and ending in July 2019 at the World Chemistry Congress and IUPAC General Assembly, we will honor a diverse group of 118 outstanding younger chemists from around the world who in embody the mission and core values of IUPAC. The resulting periodic table will highlight the diversity of careers, creativity, and dedication of the young chemists

leading us into the next century. Winners will be profiled on the IUPAC100 website and will receive a certificate from IUPAC. Elements of the Periodic Table of Younger Chemists will be revealed over time in order of scientific discovery (see Wikipedia). Approximately eight elements will be revealed each month beginning in July 2018 with the final elements being awarded at the IUPAC General Assembly and World Chemistry Congress in Paris, France in July, 2019, https://iupac.org/100/pt-of-chemist/.

THE PERIODIC TABLE CHALLENGE

The year 2019 marks the 100th anniversary of IUPAC and also the 150th anniversary of the development of the Periodic Law of the Elements independently by Dmitri Mendeleev and Lothar Meyer. To celebrate these anniversaries, IUPAC is hosting an online challenge about the Periodic Table of the Elements aimed at a global audience of young students. Our goal is to reach players from every country. The challenge runs from January 2019 and will be available all year until the end of 2019.

The IUPAC Periodic Table Challenge will present you with 15 randomly chosen multiple-choice questions about the elements. To play, you will be asked to choose an element as avatar. Your score will go towards this element in the leaderboard. When you finish the challenge, you will be asked to provide your name and **E-mail** so we can keep track of your achievements. Please enter your name and **E-mail** after finishing the Challenge: without it your efforts will not reach us. The Challenge is in English and if you have difficulties in understanding some of the questions, please copy the text and use online translation tools to help. Share your experiences on social media using #PeriodicTableChallenge or #iupac100, https://iupac.org/100/pt-challenge/.

ORGANIZATION

The IUPAC Council will meet in Paris in July 2019. Actions from last meeting in São Paulo, Brazil July a 2017 along with the IUPAC Bureau. The following actions were taken by the Bureau: https://iupac.org/actions-taken-iupac-council-bureau-sao-paulo-brazil-2017/.

Summary of some actions:

Election of the Officers. On 1 January 2018, Qi-Feng Zhou (China), Vice President and President-Elect of IUPAC, will become President. Natalia Tarasova (Russia), current President, will become Past President and remain an officer and a member of the Bureau for a period of two years. Meanwhile, Marc Cesa (USA), current Past President, will retire. Secretary General Richard Hartshorn (New Zealand) and Treasurer Colin Humphris (UK) were both elected by the Council in August 2015 for a four-year term and will continue their service for two more years.

The candidates for Vice President were Professor Christopher M.A. Brett (Portugal) and Professor Javier García Martinez (Spain). Christopher M.A. Brett was elected.

Council formally adopted the Recommendations approved by the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) and published in Pure and Applied Chemistry from August 2015 through June 2017.

Council ratified the decision of Bureau for the names and symbols of the four new elements, Z = 113, Z = 115, Z = 117, and Z = 118.

Council approved designation of the International Younger Chemists Network as an Associated Organization of the Union.

Council ratified the Executive Committee's decision to establish the Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD) and approved the proposed Terms of Reference of the Committee.

Council reauthorized the Commission on Physicochemical Symbols, Terminology and Units (I.1), the Commission on Isotopic Abundances and Atomic Weights (II.1), and the IUBMB- IUPAC Joint Commission on Biochemical Nomenclature (JCBN).

CITAC
Cooperation on International Traceability in Analytical Chemistry

MOST INTERESTING/ IMPORTANT PAPERS ON METROLOGY IN CHEMISTRY IN 2018

A NEW REALIZATION OF SI FOR ORGANIC CHEMICAL MEASUREMENT: NIST PS1 PRIMARY STANDARD FOR QUANTITATIVE NMR (BENZOIC ACID)

Michael A. Nelson[1], Jason F. Waters[1], Blaza Toman[1], Brian E. Lang[1], Alexander Rück[2], Kathrin Breitruck[2], Markus Obkircher[2], Anthony Windust[3], Katrice A. Lippa[1]

[1]National Institute of Standards and Technology, USA; [2]Sigma-Aldrich Production GmbH, Switzerland; [3]National Research Council Canada

INTRODUCTION AND SUMMARY

Metrological traceability for chemical measurements is a fundamental pillar of many industries and services, yet sound establishment of this property is not always straightforward in either a theoretical or practical sense – especially relationships to the International System of Units (SI). Quantitative organic chemical assays are conditioned upon the use of artifact calibrators to translate observable measurement data into meaningful results. These calibration reference materials must therefore embody reliable realizations of the relevant kinds of chemical quantities, often characterized as SI measurement units mol/kg, kg/kg etc. Theoretically, traceability of such characterizations to the SI requires complete knowledge of the material composition. While achieving this degree of insight is an unrealistic objective, SI measurement units are *practically* realized for chemical reference materials through diligent procedures for evaluating purity[1,2]. In this fashion, sound linkage between an organic chemical measurement results and SI is ultimately substantiated through *confidence* in purity characterizations.

Since there are countless unique organic chemical structures, unambiguous identification is a critical component of metrologically sound purity analyses. Quantitative nuclear magnetic resonance spectroscopy

(qNMR) is a powerful, direct measurement technique that infers chemical structure and is inherently quantitative[3,4]. With qNMR, the magnitude of analytical response for each chemical moiety in a substance is uniformly proportional to the number of corresponding resonant nuclei, allowing mole ratios of distinct structures to be evaluated without compound-specific calibration. This technique satisfies the fundamental tenets for traceable purity characterizations and is a go-to approach for producing chemical calibrators that support a vast variety of traceable chemical calibrations[13-15] for healthcare, forensic investigation, pharmaceutical development, food safety and toxicology, biomedical research, and chemical manufacturing.

One limitation of qNMR is that the amount of one chemical moiety cannot be determined absolutely without comparison to the known amount of another, and a primary reference standard is required to transfer realization of SI measurement units for another substance. Historically, acidimetric primary standards, such as the National Institute of Standards and Technology (NIST) Standard Reference Material (SRM) 350b Benzoic acid (Acidimetric), have been used for this purpose because they have SI-traceable chemical characterizations (H^+ coulometry), contain chemicals with measurable ^1H content, and are very pure (mass fraction>99.99 %)[5]. Coulometric acidimetry is a primary measurement technique founded on Faraday's Laws of Electrolysis and does not require chemical calibration to determine quantities (mol/kg) of H^+ that are traceable to SI units for mass (kg), amount of substance (mol), electrical current (A) and time (s).

Unfortunately, acidimetry is not selective for organic molecules and H^+ elicits a measurable response regardless of provenance. Units realized through this method are distinct from those of complete chemical structures (e.g. benzoic acid). As such, a traceability gap exists for qNMR purity procedures using these primary standards due to lack of demonstrable confidence that the relative amount of H^+ is stoichiometrically congruous with that of the entire chemical structure.

Furthermore, molecular weight must be known to convert the realized H^+ amount content (mol/kg, formally "massic amount[6](" to mass fraction (kg/kg) of benzoic acid. Though the associated uncertainty can be calculated according to guidelines provided by the International Union of Pure and Applied Chemistry (IUPAC) Commission on Isotopic Abundances and Atomic Weights (CIAAW), stable isotope ratios and elemental composition can vary significantly amongst different real materials[7]. Measurement of actual stable isotope ratio content for a qNMR primary standard is critical because 1) it is an inherent aspect of the stated chemical identity, 2) a full accounting of the uncertainty of mass fraction purity is required for SI traceability, and 3) only ^1H, not ^2H, nuclei are observable via ^1H-NMR.

To close this gap in metrological traceability, the National Institute of Standards and Technology (NIST), in coordination with Sigma Aldrich Production GmbH and the National Research Council Canada (NRC), has developed a reference material intended explicitly for use with qNMR – the NIST PS1 Primary Standard for quantitative NMR (Benzoic Acid). Given that qNMR is a preferred technique for purity assessment of neat chemical materials, NIST PS1 directly supports production of other calibrators that can in turn be implemented to establish SI-traceability for the measurement of countless distinct organic chemical species. Multiple primary measurement techniques, including coulometric acidimetry and qNMR, instilled confidence that the SI-traceable quantification of H^+ content in NIST PS1 is consistent with that inferred for the benzoic acid molecular entity and corresponding mass fraction. This confidence, also supported by precise determination of molecular weight and an investigation of impurities, substantiated realization of SI measurement units for amount content (mol/kg) and mass fraction (kg/kg) of benzoic acid.

EXPERIMENTAL RESULTS AND CONCLUSIONS

NIST PS1 is comprised of crystalline benzoic acid, manufactured and packaged into individual 1 g units by Sigma-Aldrich Production GmbH (Buchs, CH). This material was jet milled (Jetpharma SA, Balerna, CH) prior to bottling to release occluded water.

Complete-structure inferences of purity were achieved

through H^+ coulometry, ^{1}H-qNMR using an internal standard (^{1}H-qNMR$_{IS}$), ^{1}H-qNMR using an external standard (^{1}H-qNMR$_{ES}$), and an indirect mass balance approach (1-$\sum w_{impurites}$). Ratios of H, C, and O stable isotopes were measured at the U.S. Geological Survey Reston Stable Isotope Laboratory.

Molecular Weight Relative atomic masses were derived from measured δ^{13}C, δ^{2}H, and δ^{18}O relative to VPDB and VMSOWSLAP and used to calculate the relative molecular mass 122.12204 (u=0.00019)[8]. This is used to convert mol/kg of benzoic acid to mass fraction. Independent confirmatory determinations of δ^{13}C were made by the NRC.

Coulometric Acidimetry SI traceable assays of H^+ were conducted for 34 units of PS1 using constant-current coulometric generation of hydroxide[9]:

$$OH^- + C_6H_5COOH \rightarrow H_2O + C_6H_5COO^-.$$

The mass fraction (W_p) of benzoic acid was evaluated using Eq. 1

$$W_P = \frac{MIt}{m_p nF} \quad (1)$$

where M is the calculated molecular weight; I is titration current; t is titration time; m_p is the sampled mass; n is the charge number (moles of electrons per mole of analyte oxidized), and F is the Faraday constant, 96485.33212 C mol^{-1}. Mass purity was determined to be W_P 99.9923% ±0.0040% ($U_{95\%}$, k=1.97).

^{1}H-qNMR$_{IS}$ Ten units of PS1 were evaluated using qNMR with independent comparison to four chemically-distinct internal standards: 1) dimethyl sulfone, 2) 2,2-dimethylpropanedioic acid, 3) 3,5dinitrobenzoic acid, and 4) maleic acid, which were calibrated by qNMR comparison with NIST SRM 350b Benzoic Acid and SRM 84k Potassium Hydrogen Phthalate. This experimental design accounts for statistical correlation of results to individual reference materials. ^{1}H-NMR experiments were performed using a spectrometer operating at 600.14 MHz and with 90° singlepulse excitation sequences without ^{13}C decoupling. Spin-lattice relaxation times (T_1) of benzoic acid and internal standard resonances were evaluated and recycle delays at least 12x the longest T_1 were used for all experiments. Purity was calculated using an observation equation approach under the Bayesian paradigm[10,11]. This approach accounted for uncertainty of measurement function variables (bottom-up) and random effects associated with repeatability and experimental design (top-down). Results were constrained below the natural limit 1 (g/g). A hierarchical model was used to calculate a result based on all four internal standards (Figure 1) with a value and 95% confidence interval, 99.992%, $U_{95\%}$ = [99.981, 99.997]%. Consistency of results using different internal standards improves confidence in the qNMR result accuracy and that certified values of SRM 350b and SRM 84k calibrators are congruous with the respective organic chemical purities and natural abundance of ^{1}H isotopes.

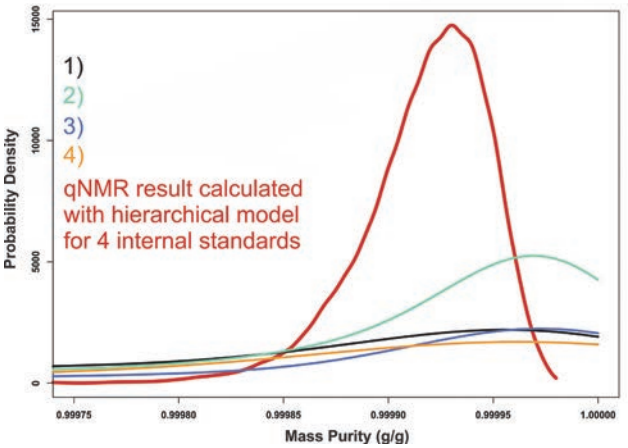

Figure 1 Purity results of 1H-qNMRIS measurements using four internal standards

^{1}H-qNMR$_{ES}$ Five units of PS1 were evaluated using a qNMR external standard procedure for comparison with solutions of SRM 350b Benzoic Acid (Acidimetric)[12]. The 95% confidence interval of this result lies between 99.4% and 100%. This direct comparison supports metrological traceability of the certified value of SRM 350b Benzoic Acid for historical use with qNMR.

1-Σ Impurities Low water content (0.0041% ± 0.0015%), determined via Karl Fischer titration, and non-volatile ash content (0% - 0.0012%) were quantifiable impurities. No structurally related or other impurities were detected via liquid chromatography with high resolution mass spectrometry or 1D and 2D NMR experiments. The 95% confidence interval of purity through this method lies

between the values 0.99983 kg/kg and 0.99997 kg/kg. This approach provided confirmatory information to support the confidence in certified values.

Certified values and Measurement Uncertainty Certified values of NIST PS1 are based on a Bayesian consensus, constrained below 1 kg/kg, that blends the coulometry and ^{1}HqNMR$_{IS}$ estimates and treats both techniques as equavalent indicators of purity. The consistency of results determined from each orthogonal technique (Figure 2) provides unequivocable confidence that the SI units realized for NIST PS1 are relevant for the entire benzoic acid molecular entity.

Table 1 NIST PS1 certified values for benzoic acid chemical purity and amount content

	kg/kg[1]	mol/kg[1]
1	0.99992 -0.00006 + 0.00004	8.1880 -0.0005 + 0.0004

[1] Expressed as $-U_{L95\%}+U_{H95\%}$ where x denotes the certified value and $U_{L95\%}$ and $U_{H95\%}$ indicate the lower and upper boundaries of the 95% coverage interval

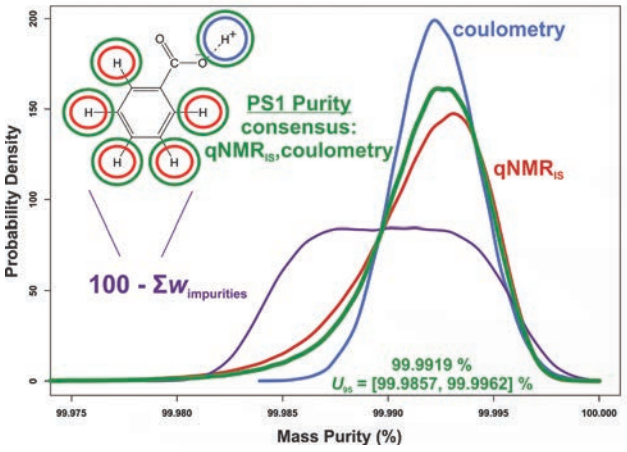

Figure 2 Probability density distributions of benzoic acid mass purity determined from coulometry, qNMR$_{IS}$, coulometry-qNMR$_{IS}$ consensus, and investigation of impurities

The NIST PS1 will serve as a pinnacle reference standard for metrological traceability chains, establish the highest order of comparability, and promote accuracy for quantitative measurements across the organic chemical sector. This will directly impact services and deliverables for many industries, and through SI-traceability, these communities can produce more reliable measurements that are consistently meaningful across time and place.

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SUMMARY OF "PURITY ASSIGNMENT FOR PEPTIDE CERTIFIED REFERENCE MATERIALS BY COMBINING QNMR AND LC-MS/MS AMINO ACID ANALYSIS RESULTS: APPLICATION TO ANGIOTENSIN II"

Anal. Bioanal. Chem., Vol. 410, 2018, p. 6719-6731

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National Research Council Canada, Metrology

INTRODUCTION

Unlike small organic molecules that can be readily synthesized and isolated with high chemical purity, peptides are difficult to prepare as high-purity standards. The wide range of functional groups and multiple charge sites of peptides typically result in significant co-crystallization of counter-ions or salts [1]. If measured by conventional means, such as LC-UV, the amount of these salts can be greatly underestimated [1]. Therefore, the purity value assignment of metrologically traceable peptide reference standards requires specialized primary methods. Conventionally, amino acid analysis by isotope dilution tandem mass spectrometry (LC-MS/MS) following peptide hydrolysis is employed as a reference method[2]. By contrast, quantitative nuclear magnetic resonance (qNMR) spectroscopy allows for quantitation of intact peptides, thus eliminating potential bias due to hydrolysis. Both methods are susceptible to interferences from related peptide impurities, which need to be accurately accounted for. The mass balance approach has also been employed for peptide purity measurements[3], whereby the purity is defined by the sum of the mass fractions of all impurities identified.

In this summary of the original article published in Analytical and Bioanalytical Chemistry [4], we describe a comprehensive workflow for a metrologically traceable determination of simple linear peptides. The workflow is demonstrated with the value assignment for a candidate NRC certified reference material for angiotensin II (ANGII-1), and summarized in Figure 1.

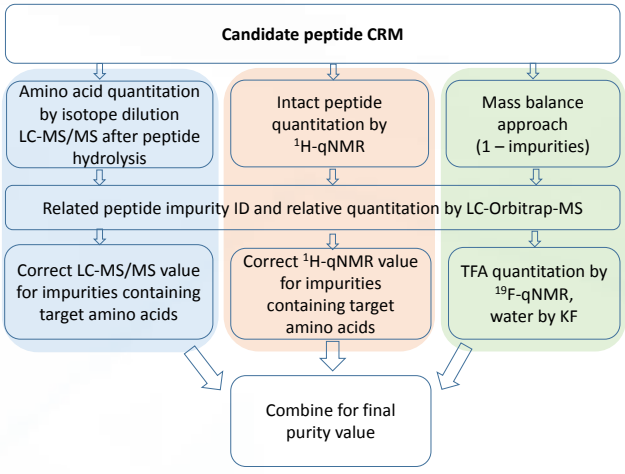

Figure 1. Workflow used for purity (mass fraction) value assignment for candidate peptide CRMs.

SUMMARY OF RESULTS

Amino acid analysis by LC-MS/MS

The amount fractions of Pro, Val, and Phe were determined in three independent samples of ANGII-1 by LC-MS/MS. Given the equal unit stoichiometry of these four amino acids in the Ang II sequence, the resulting amount fractions should be identical. The results yielded good agreement between Pro, Val, and Phe with values of 0.671 mmol/g (u = 0.006 mmol/g) for Pro, 0.646 mmol/g (u = 0.006 mmol/g) for Val, and 0.668 mmol/g (u = 0.005 mmol/g) for Phe from the 2016 measurement campaign based on three independent ANGII-1 sample analyses, each in triplicate.

Angiotensin II quantitation by ^{1}H-qNMR

Significant preliminary qualitative NMR analysis was performed to assign angiotensin II signals suitable for quantitative use, and the two aromatic signals of Tyr were selected (Fig. 2), namely the signal at 6.67 ppm signal corresponding to the 2′ and 6′ aromatic protons and the signal at 7.01 ppm corresponding to the 3′ and 5′ aromatic protons, as depicted in Fig. 2.

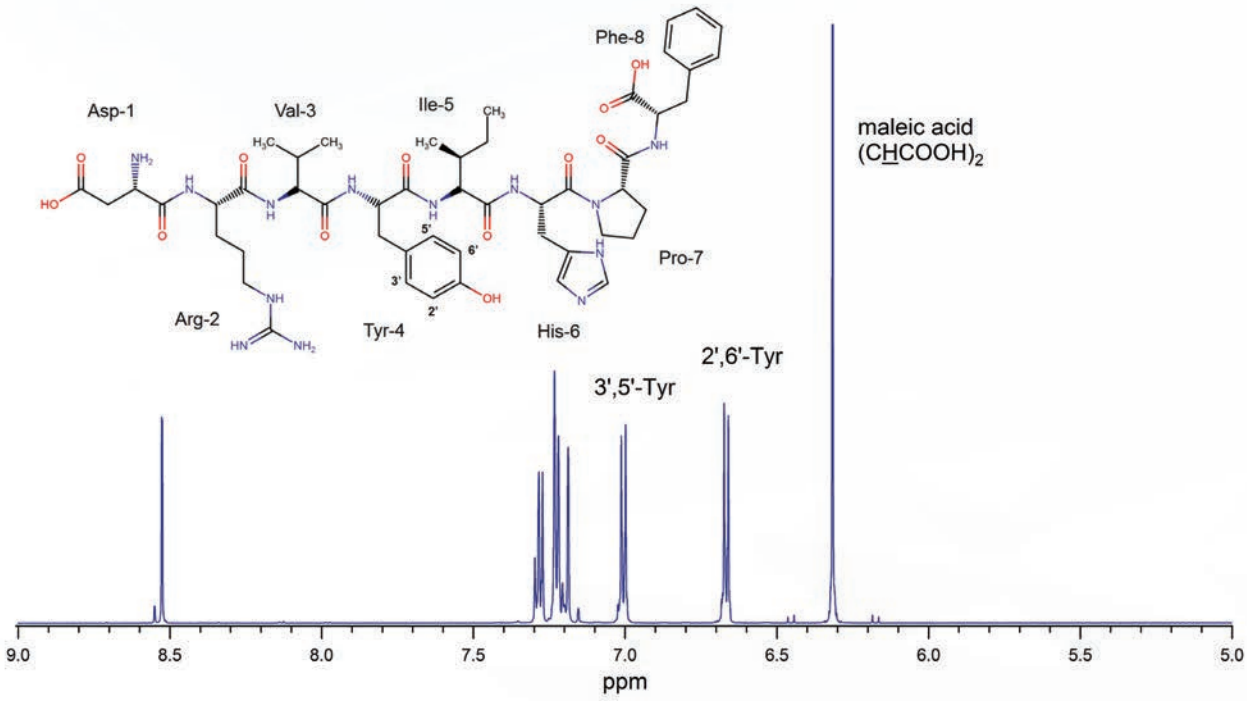

Figure 2. Quantitative ^{1}H-NMR spectrum of angiotensin II with maleic acid internal standard, showing the region used for quantitation. The two sets of two equivalent aromatic protons of tyrosine are indicated. The full spectrum of angiotensin II is shown in Figure S1.

The choice of internal standard was then considered and maleic acid was selected owing to its solubility in D_2O and the lone ^{1}H-NMR signal at 6.3 ppm from its two vinyl protons. The maleic acid signal lies in a void region of the Ang II spectrum and thus offers interference-free integration required for accurate quantitation. Using this method, amount fractions measured for Tyr during the 2016 measurement campaign were as follows: 0.6712 mmol/g (u = 0.0035 mmol/g) for the 6.67 ppm signal and 0.6714 mmol/g (u = 0.0020 mmol/g) for the 7.01 ppm signal, based on three independent ANGII-1 sample analyses, each in triplicate.

Trifluoroacetic acid quantitation by ^{19}F-qNMR

Trifluoroacetic acid (TFA) is used during solid-phase peptide synthesis and is typically the resulting counter-ion following peptide purification. Therefore, it can be present at significant levels in synthetic peptide samples and is generally not considered in the LC-UV based purity estimates quoted by most peptide manufacturers. TFA was thus measured by ^{19}F-qNMR using a procedure that was validated against established ion-chromatography

methods in an international laboratory inter-comparison exercise [5]. A CRM of 3,5-bis(trifluoromethyl)benzoic acid was employed as internal standard, and was well resolved from the TFA signal. Using this approach, a TFA mass fraction of 248.3 mg/g (u_c = 2.3 mg/g) was obtained in the ANGII-1 samples.

Angiotensin II Peptide Impurity Analysis by LC-HRMS

Relative ESI-MS responses were used for peptide quantitation, as discussed in detail elsewhere [6]. Mass fractions derived from impurity: Ang II peak area ratios were consistent with those calculated from standard addition experiments, within the measurement uncertainties[6]. Impurity amounts ranged from 3.71 mg/g (P2b) down to 0.01 mg/g (P9), and the summed amount of all peptide impurities represented 10.8 (u = 1.2) mg/g.

Correction of amino acid analysis results (LC-MS/MS and ^{1}H-qNMR) to account for related peptide impurities

After undergoing acid hydrolysis, the ANGII-1 sample was subjected to LC-MS/MS analysis of three amino acids (Pro, Phe, and Val) using the double isotope dilution method. In addition, the amount of tyrosine was determined with ^{1}H-qNMR on the intact peptide. The amounts of these amino acids are then translated into the amount of Ang II from the stoichiometric ratio of the corresponding amino acids in the peptide sequence. However, these four amino acids may originate not only from Ang II, but also from any peptide impurities present in the solution.

Consider a sample containing angiotensin II (Ang II) and M peptides (P_1,...,P_M) of known stoichiometry. If all of these peptides are hydrolyzed to release, as an example, valine, the amount of valine released is given as

$$n(\mathrm{Val}) = z(\mathrm{Ang\ II, Val})\,n(\mathrm{Ang\ II}) + z(\mathrm{P_1,Val})\,n(\mathrm{P_1}) + \ldots + z(\mathrm{P_M, Val})\,n(\mathrm{P_M}) \quad (1)$$

where z(Ang II,Val), as an example, is the number of valine entities per molecule of Ang II. If the amount ratios of all peptide impurities to Ang II, i.e. $R(\mathrm{P_i}) = n(\mathrm{P_i})/n(\mathrm{Ang\ II})$, are known, Eq. 1 can be written as follows:

$$n(\mathrm{Val}) = n(\mathrm{Ang\ II}) \sum_{\mathrm{E}} z(\mathrm{E,Val}) \cdot R(\mathrm{E}) \quad (2)$$

where summation is over substances E = {Ang II, P_1, ..., P_M}. From here, we obtain the amount of angiotensin II:

$$n(\mathrm{Ang\ II}) = n(\mathrm{Val}) \frac{1}{\sum_{\mathrm{E}} z(\mathrm{E,Val}) \cdot R(\mathrm{E})} \quad (3)$$

The mass fraction of angiotensin II in the sample of ANGII-1 (the chemical purity) is

$$w(\mathrm{Ang\ II}) = \frac{n(\mathrm{Ang\ II}) \cdot M(\mathrm{Ang\ II})}{m(\mathrm{ANGII\text{-}1})} = \frac{n(\mathrm{Val})}{m(\mathrm{ANGII\text{-}1})} \cdot \frac{M(\mathrm{Ang\ II})}{\sum_{\mathrm{E}} z(\mathrm{E,Val}) \cdot R(\mathrm{E})} \quad (4)$$

where m(ANGII-1) is the mass of the sample and M(Ang II) is the molar mass of angiotensin II. Eq. 4 serves as the measurement model equation to determine the amount of angiotensin II in the ANGII-1 sample.

Note that the observed mass spectrometry signals are based on the monoisotopic ions so their abundances must be taken into the account when converting the mass spectrometric signal intensity ratios into the corresponding amount ratios. As an example, the monoisotopic signal for peptide impurity YIHPF comprises 65% of all isotopologues whereas the abundance of the monoisotopic ion is only 49% for DRRVYIPF [6].

COMBINING LC-MS/MS AND ^{1}H-QNMR RESULTS

Bayesian methods are gaining popularity in chemical metrology [7], including applications to chemical purity assignments using ^{1}H-qNMR [8, 9]. The Bayesian approach to uncertainty assessment allows one to consider both empirical data and pre-existing knowledge. In particular, recognizing that neither the acid hydrolysis isotope dilution methods nor ^{1}H-qNMR alone are universal methods, we find it desirable to reconcile these results with the mass balance of known impurities similar to the approach by Nelson et al. [9].

The two major impurities in ANGII-1 are TFA and water, followed by the related peptide impurities: w(TFA) = 248.3 (u = 2.3) mg/g, $w(H_2O)$ = 34 (u = 8) mg/g, and w(related peptides) = 10.8 (u = 1.2) mg/g. Together, these known impurities provide a total mass fraction of

$w_{\mathrm{total}} = w(H_2O) + w(\mathrm{TFA}) + w(\mathrm{related\ peptides}) = 293$ (u = 9) mg/g.

Assuming that these impurities constitute an exhaustive list of foreign substances in ANGII-1, the Ang II content

can be estimated using the mass balance ('one minus') approach as

$$w(\text{Ang II}) = 1 - w_{\text{total}} = 707\ (u = 9)\ \text{mg/g}$$

This value is consistent with the maximum likelihood consensus estimate of w(Ang II) = 690.3 (u = 2.4) mg/g at 95% confidence level. This indirect mass balance estimate of Ang II is then blended with the IDMS and ^{1}H-qNMR results of Ang II using Bayesian methods. Briefly, the mass balance result (normal distribution with mean 707 mg/g and standard deviation 9 mg/g) serves as the prior knowledge of w(Ang II) along with weakly informative prior information regarding the between-method uncertainty (modeled as half-Cauchy distribution with median 70 mg/g corresponding to 10% relative uncertainty) as shown in Fig. 3. We also compare this result with Bayesian method using weakly informative priors for the consensus mean.

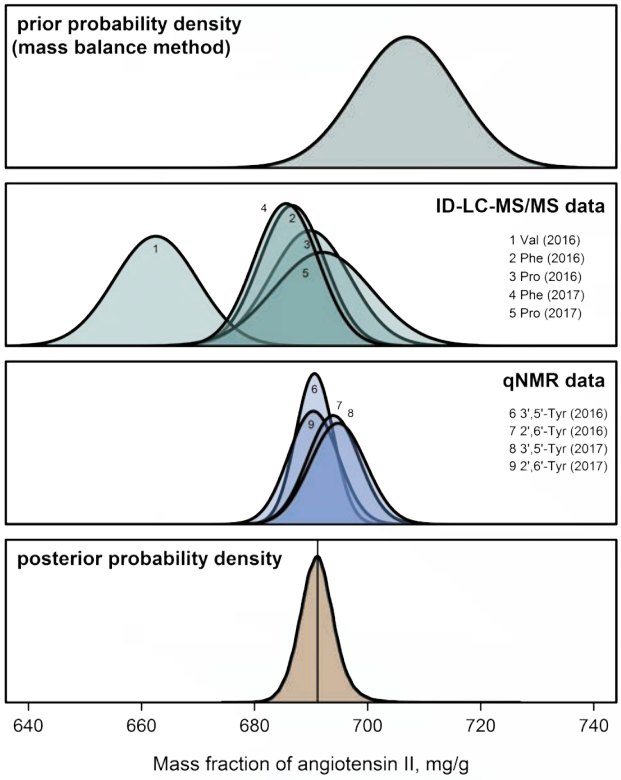

Figure 3. Bayesian combining of IDMS, ^{1}H-qMNR, and mass balance results for consensus estimate of the Ang II content in ANGII-1 certified reference material. (The 2017 valine result is omitted from the graph due to its large uncertainty).

CERTIFIED VALUE ASSIGNMENT AND UNCERTAINTY EVALUATION

Based on the consensus mass fraction of Ang II described above, a certified value w(Ang II) = 691 mg/g was assigned with an expanded uncertainty U=9 mg/g. Included in the combined uncertainty estimate (u_c) are uncertainties in the batch characterization (u_{char}), uncertainties related to possible between-bottle variation (u_{hom}), and uncertainties related to stability ($u_{stability}$). Expressed as standard uncertainties, these components are listed in Table 1. The small relative uncertainty (< 1 %) is a reflection of the high metrological rigour of the proposed workflow.

Table 1. Summary results for the angiotensin II content in ANGII-1

w(Ang II), mg/g	U (k=2) mg/g	U_c mg/g	U_{char} mg/g	U_{hom} mg/g	U_{stab} mg/g
691	9	4.7	3.3	3.3	0.0

CONCLUSIONS

A comprehensive workflow for the purity value assignment of reliable peptide reference standards has been described. Our method incorporates a simple, yet accurate, approach for the correction of the LC-MS/MS and ^{1}H-qNMR results for amino acid interferences originating from related peptide impurities in the sample. Despite both methods providing reliable and consistent results, it is useful from a practical standpoint to establish a purity ceiling by tallying the amounts of all known impurities. Therefore, the mass balance approach serves as a benchmark for the direct methods and Bayesian methods of data reduction are well suited to blend this prior knowledge about the peptide purity with the results from both direct methods of analysis.

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SI TRACEABILITY AND SCALES FOR UNDERPINNING ATMOSPHERIC MONITORING OF GREENHOUSE GASES

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INTRODUCTION

We consider two approaches for a measurement system for greenhouse gas amount-of-substance fractions (later referred to as amount fraction) in the atmosphere. The first provides traceability to the International System of Units (SI) and the second to a defined scale. We consider the advantages and disadvantages of each approach and how the measurement system may ultimately benefit from an approach that combines elements of each.

DISCUSSION

In the field of gas analysis, reference materials are usually disseminated in high pressure cylinders using gravimetric methods to assign the reference value. There is a broad consensus amongst metrologists that 'verification' is required to ensure the 'primary method' is behaving as expected [1]. The implication is that within gas metrology, amount fraction values can be realised and their uncertainties calculated with traceability to the mole. This is achieved via mass and purity measurements, tables of atomic weights and the molar mass constant *Mu*. These values should then be verified by comparison against an independently prepared gas mixture of similar composition. This process is intended to demonstrate that errors in preparation, loss of material to cylinder walls, and reaction of gas components within the mixture are well understood. It is agreed that this verification step provides a good demonstration that the value and uncertainty have been properly assigned, based on a gravimetric value fully traceable to the SI [2]. The general methods for the realisation of gas standards with assigned amount fractions is described within the written standard ISO 6142-1:2015 [2]. This methodology has been successfully used by NMIs to develop standards for greenhouse gases for different measurement communities from emission levels down to background atmospheric levels and below.

An alternative approach is a measurement system based on traceability to a "scale", often a family or collection of gas standards, based on an agreed reference value or reference method. This system offers superior precision as comparisons are made to one source and the absolute accuracy of the artefact has limited impact on measurement compatibility, provided that all measurements are traceable to the same reference, and that reference is stable. Within the greenhouse gas field (particularly at the global scale), this practice arose partially out of the realisation that gas amount fraction measurements could be performed with precisions that were often better than the uncertainties associated with gas mixture preparation. In addition, the key quantity to be measured was the relative difference in amount fraction between different measurement sites within a network. A fundamental characteristic of the scale approach is that a scale, once defined, is intended to serve as a fixed reference over a specific amount fraction range. For greenhouse gas analysis, a scale is often defined by a series of gas mixtures, prepared gravimetrically or otherwise, with amount fractions that span the range of scientific interest. The standards are typically value assigned by methods that can provide SI traceable values and associated measurement uncertainties. However, the ensemble of standards is then used to define a calibration curve. It is this calibration curve which is taken to be the stable reference for the scale. The stability of the scale and small uncertainties that can be achieved for subsequent calibrations in the traceability chain, then permit different laboratories to achieve metrological compatibility of measurements.

Using the scale approach, the level of compatibility of measurements is typically lower than can be achieved for individual primary standards alone. For example, the uncertainty associated with primary carbon dioxide standards in the ambient range measured by the National Oceanic and Atmospheric Administration (NOAA), using the manometric method is ~0.2 μmol mol^{-1} (k=2). However, the reproducibility of value assignments made relative to a fixed scale is about a factor of three better using a non-dispersive infra-red (NDIR) method [3], and a factor of ten better using a spectroscopic method. [4]. Maintenance of a scale requires intensive and uninterrupted effort generally at one location or one institute, as drift in the reference artefact would have significant implications. Because a scale is typically defined by the entire collection of gas standards, removing or adding artefacts to the collection could result in a measurable difference between sets. Thus, scales are identified by name, and included in WMO/GAW metadata. Changes are documented when significant at the level important for the scientific application.

SI traceable values are rarely corrected, or shifted, unlike scale values as it is assumed that the uncertainty covers the 'true value'. In addition, key comparisons for the major greenhouse gases are being run by sending standards for comparison measurements to one central laboratory, which allows the reference value for cylinders to be

calculated from the largest consistent set of standards. This has had the advantage of reducing uncertainties of the reference value with the expectation that a future repeat comparison would produce reference values that agreed with previous comparison results within the stated uncertainties.

Within a network using the scale approach, Data Quality Objectives (DQOs) are set, of which compatibility goals are a subset. The most current definition of compatibility within this setting is taken from the report of the 18th WMO/IAEA Meeting on Carbon Dioxide, Other Greenhouse Gases and Related Tracers Measurement Techniques (GGMT-2015) [5], in which it is defined as a property of a set of measurement results, such that the absolute value of the difference between any pair of measured values from two different measurement results is within a chosen value which does not have to be the same as the total combined uncertainty. The GGMT-2015 and VIM definitions of compatibility are significantly different, with the GGMT-2015 definition, not comparing differences in results to magnitudes of measurement uncertainties. Further guidance on determining compatibility of measurement results within a network are expected to be developed, including further clarification as to whether compatibility goals should be considered as limit values or as 1 sigma values for a distribution of differences measured, both having been previously reported [5, 6].

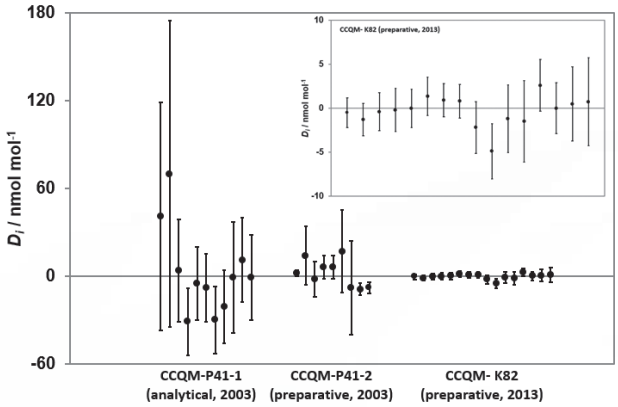

Figure 1 Results of the last three international CCQM key comparisons for assessing the analytical and preparative capabilities of NMIs for measuring methane in an air matrix. Bars show expanded uncertainties.

The accuracy of the scale approach has been verified by the participation of NOAA in key comparisons under the CIPM MRA as a designated institute of the WMO. Figure 1 shows the results of three comparisons organised by the CCQM Gas Analysis Working Group. The first (CCQM-P41 part 1) [7] was organised by the Van Swinden Laboratorium (VSL) in 2003 and assessed the analytical capabilities of laboratories for 1.8 μmol mol^{-1} methane and 365 μmol mol^{-1} carbon dioxide (full complement of results not presented here) in an air matrix. CCQM-P41 part 2 [8] was coordinated by VSL in the same year and assessed the preparative capabilities of laboratories for methane and carbon dioxide (full complement of results not shown here) in air at the same amount fractions as part 1. Ten years later, a third comparison coordinated by the BIPM and NIST (CCQM-K82) [9], which assessed the preparative capabilities of laboratories for the same mixture composition as CCQM-P41, resulted in standard uncertainties for reference values of 0.7 nmol mol^{-1}. Within each of these comparisons, the key comparison reference value is considered to be the best estimate of the SI traceable value and uncertainty that can be demonstrated for the amount fraction (x) measured. At the same time the result produced by NOAA or results traceable to the NOAA maintained scale, provides an estimate of the scale value (x_{scale}) and allows the difference between the two (x - x_{scale}) and their combined uncertainty to be calculated, and is depicted in Figure 2. This demonstrates a number of key issues:

a) The uncertainties in the plotted differences have historically been large when compared to the magnitude of the WMO-GAW network compatibility goals for data. There are two factors that have contributed to this, notably the magnitude of the uncertainties in the standards themselves, and the way the comparison has been performed. As can be seen from the results of the most recent comparison in 2013 (CCQM-K82) for methane, both of these issues are being addressed [9, 10]. Comparisons are now carried out in a central laboratory (BIPM), allowing the standards to be compared under repeatability/intermediate reproducibility conditions, resulting in the analytical measurement uncertainty component of the comparison to be much reduced. Secondly, the uncertainty of the standards has been reduced, particularly the verification uncertainty

component which may have been too conservative in previous comparisons.

b) In 2003 a significant bias between the SI and methane amount fraction scale value existed [11] and was corrected for in the change from the CMDL83 and NOAA04 scale for methane. However, even though a bias existed between CMDL83 and NOAA04, the CMDL83 was propagated with low uncertainty, as can be seen by the close agreement of CMDL83 as represented by two different laboratories (NOAA and CSIRO). A much smaller residual bias between the NOAA04 scale and SI value for methane was revealed in 2013.

c) There is consistency among these NMIs for carbon dioxide and methane, although uncertainties are high for the former. The quantities x-x_{NIST} and x-x_{NPL} are relatively consistent between CCQM-P41 and CCQM-K52, and between CCQM-P41 and CCQM-K82, as are the relationships between the laboratories shown in figure 2 (a) and (b).

An SI traceable measurement system could be implemented with benefits for the greenhouse gas community, if the uncertainties in the measurements standards contributed in a negligible way to the uncertainty of measurements performed at measurement sites. In comparing the magnitudes of network compatibility goals and uncertainties in the values of standards (since uncertainties are added in quadrature) this would mean that a standard uncertainty one quarter the magnitude of a compatibility goal would increase the standard deviation of the measurement results by less than 5%, and would be negligible (indeed it could be argued that standards with uncertainties one third of the size of the compatibility goals would have negligible impact on meeting them). This assumes that compatibility goals are 1 sigma for a distribution of differences measured. Returning to the example of the scale for carbon dioxide measurement, NMIs would need to demonstrate comparability and achieve measurement uncertainties substantially lower than the WMO Global Atmosphere Watch (GAW) programme's compatibility goals (which translates to a standard uncertainty in the value of the primary standard of ~25 nmol mol^{-1} for the remote northern hemisphere) to ensure that

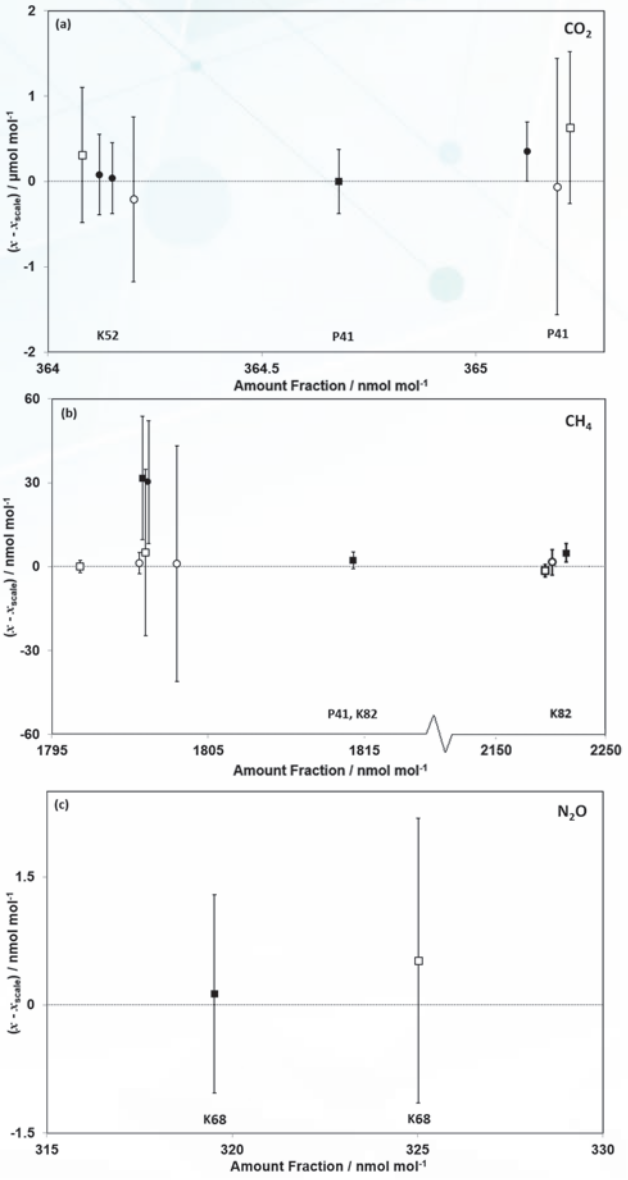

Figure 2: Estimate of differences between SI and WMO NOAA (filled squares) and WMO CSIRO (filled circles) scale, SI and NIST (open squares), and SI and NPL (open circles) traceable amount fractions for carbon dioxide, methane and nitrous oxide ((a), (b) and (c) respectively), based on results in CCQM-P41, CCQM-K52, CCQM-K82 and CCQM-K68 comparisons. Different WMO scales (filled symbols) are shown in panel (b): values at 1814 and 2214 nmol mol^{-1} are on the WMO-X2004 methane scale developed at NOAA based on gravimetrically prepared primary standards, while the value at 1801 nmol mol^{-1} is on the CMDL83 scale, which was based on two standards obtained from Biospherics (Portland, OR) [22]. In panel (a), the WMO scale naming convention for CO_2 was not formally adopted at the time of the comparisons shown. Carbon dioxide results are broadly consistent with scale WMO-X2001. NOAA results in panel (c) are on the NOAA-2006 scale.

interchangeability of reference standards would not impact on global measurements [12]. They would also need to provide stable reference standards as long-term trend detection fundamentally relies on the reference not changing with time.

The benefits of moving to SI traceability would mean

that measurements are consistent with measurements made in other areas of science and technology and can be combined easily with the measurements in more complex calculations, for instance in climate modelling. Aspects of both approaches have been adopted by NMIs and laboratories that propagate scales. For example, NOAA has made efforts to provide uncertainty estimates following accepted methods used by NMIs [13] and has participated in Key Comparisons on behalf of the WMO. In concert, some NMIs have adopted aspects of the scale approach, such as using a fixed set of SI traceable primary standards anchored to performance in a key comparison to define "scale". Those primary standards are in turn used to value assign secondary (or working) standards that remain within the NMI, to propagate that "scale". This is different from the general approach used by NMIs in value assigning secondary reference materials using primary standards. In the general case, secondary reference materials are typically available to the public sectors. In these cases, NMIs can offer batch assigned (or certified) reference materials where the level of uncertainty is not as demanding or required. However, where very tight uncertainties are required, for instance to meet WMO compatibility goals, individually analysed reference materials with a higher degree of compatibility are offered [14]. These efforts, together, should provide improved support for gas analysis to meet the requirements for atmospheric monitoring.

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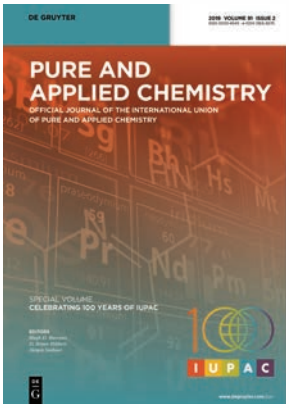
JOURNALS IN PURE AND APPLIED CHEMISTRY

PURE AND APPLIED CHEMISTRY AND THE IUPAC CENTENARY CELEBRATIONS

Hugh D. Burrows // PAC Scientific Editor



This year, the International Union of Pure and Applied Chemistry (IUPAC) is celebrating the centenary of its creation. It was founded just after the end of the First World War with the goals of promoting cooperation between the Chemical Societies of the member countries and establishing a common language for chemical researchers worldwide. One of the highlights of this year's celebrations will be the 47th IUPAC World Chemistry Congress and 50th General Assembly, to be held at the *Palais des Congrès* in Paris, France from 5th to 12th July. However, various other activities will also mark this important anniversary. We will highlight some aspects related to the IUPAC journal, *Pure and Applied Chemistry.*

In its first half-century of existence, IUPAC did not have a systematic policy on publication of reports or papers prepared by its various Commissions, Sections and Divisions. Instead, these were published through various scientific journals and societies. However, the limitations of this were recognized by the Union, and led to the creation in 1960 of *Pure and Applied Chemistry* as the official journal of IUPAC, with H. W. Thompson (University of Oxford, UK) as Chairman of the Editorial Advisory Board. This was published by Butterworth & Co., and the first volume featured papers from the *Radioactivation Analysis Symposium* held in Vienna, Austria in June 1959, together with various Recommendations from the IUPAC section on Analytical Chemistry, and Commission on Molecular Structure and Spectroscopy. In the early years of *PAC*, papers were published in English, French and German. However, as the journal evolved, English became dominant. In addition, the publication schedule developed from the initial publication of various volumes each year up to the late 1970's, when it started to be published in its current format as 12 monthly issues in a single annual volume.

Pure and Applied Chemistry (PAC) is now an important, widely read and cited publication. It publishes high quality peer-reviewed works arising from those international scientific events and projects that are sponsored and undertaken by the Union. These include papers based upon Plenary, Keynote and Invited Lectures presented at IUPAC endorsed conferences, symposia and workshops, invited papers or collections of papers as special topic features, IUPAC Recommendations on

nomenclature, symbols and units, and IUPAC Technical Reports on standardization, recommended procedures, collaborative studies, data compilations, etc. The policy of *PAC* is to publish highly topical and credible works covering all aspects of pure and applied chemistry, with the goal of promoting acceptance of the Journal as an authoritative and indispensable holding in academic and institutional libraries. To ensure high quality of publication, all manuscripts re rigorously peer reviewed. *PAC* is in the first quartile of journals in the category of multidisciplinary chemistry, with a current Impact Factor of 5.294, and 5-Year Impact Factor of 3.350 (Web of Science Journal Citation Reports). While bibliometric parameters can be misleading. The scientific level of the journal is indicated by the fact it currently has 15 "Highly cited papers" (papers that have received enough citations to place it in the top 1% of the academic field of Chemistry based on a highly cited threshold for the field and publication year).

PAC is published monthly in partnership with De Gruyter, both online (degruyter.com/pac) and in print. As soon as accepted manuscripts have been prepared for publication they are available "Ahead of Print" on the journal's website. The Editors are, currently, Jürgen Stohner, D. Brynn Hibbert (IUPAC Technical Reports and Recommendations), and myself (Scientific Editor, Conference and Special Topic Papers). The journal has an Editorial Advisory Board, chaired by the IUPAC Secretary General, Richard Hartshorn, and including representatives of all the IUPAC Divisions, the Editors, together with the chair of the IUPAC Committee on Publications and Cheminformatics Data Standards, Bonnie Lawlor.

As has been highlighted in a recent Editorial (B. Lawlor, R. D. Weir, H. D. Burrows, *Pure Appl. Chem.* 2017, **89**, 1737-1738) *Pure and Applied Chemistry* strongly supports Open Access. IUPAC Standards and Recommendations are internationally-binding for scientists in industry and academia, and the Union believes that this information must be freely-accessible, not only for the benefit of science, but also for the benefit of society in general. These papers are, therefore, Open Access upon publication. Conference and Special Topic papers normally become Open Access after 2 years.

Special Topic issues are devoted to rapidly developing areas which are likely to be of general interest. In 2018, we published two of these on "Chemistry and Cultural Heritage" and "Innovative Technologies for Chemical Security (Chemical Weapons Convention)".

To celebrate the IUPAC Centenary, *Pure and Applied Chemistry* is being published this year with a special cover. In addition, our publication schedule will reflect this special anniversary. In addition to the continuing publication of IUPAC Technical Reports and Recommendations, we intend to feature selected papers from the 47th IUPAC World Chemistry Congress, as well as the presentations from various conferences, including ones on Polymers and Organic Chemistry, High Temperature Materials Chemistry, Chemistry for Beauty and Health Conference, Global Challenges in Neglected Tropical Diseases, Physical Organic Chemistry, Solubility Phenomena and Related Equilibrium Processes, Eurasia Conference on Chemical Sciences, Solid State Chemistry, Bioinspired and Biobased Materials, Carbohydrate Chemistry. An issue, will be devoted to papers from the winners of the 2018 IUPAC- Solvay International Award for Young Chemists. In addition, a particular highlight of this year will be the publication of two issues devoted to contributions from women who have received the IUPAC Distinguished Women in Chemistry and Chemical Engineering Award. These take the form of short scientific or technical reviews, as well as career advice for young scientists and engineers.

As well as this being the Centenary Year of IUPAC, the General Assembly of the United Nations has proclaimed 2019 as the International Year of the Periodic Table of Chemical Elements. As part of the celebrations, *Mendeleev 150: 4th International Conference on the Periodic Table* will be held in St Petersburg, Russian Federation from 26th to 28th July. Papers from this will be published in *Pure and Applied Chemistry.*

I hope that this has given a taste of what to expect from *PAC* in this IUPAC Centenary Year. However, anniversaries are like buses; you wait a long time for one and then two come around the same time. Next year (2020) will be the 60th anniversary of *Pure and Applied Chemistry.* Expect more news on this soon!

CHEMISTRY INTERNATIONAL 2019 AT THE INTERSECTION OF IYPT & IUPAC100

Fabienne Meyers // CI Managing Editor

It is not every year that our calendar seems as festive as 2019. Of interest to chemists, 2019 will see the celebrations of the International Year of the Periodic Table of Chemical Elements (IYPT) and of the 100 years anniversary of the Union, flagged with activities and events scattered over the year. *Chemistry International (CI),* as the magazine of International Union of Pure and Applied Chemistry (IUPAC), will follow suit and its content will embrace the opportunities to celebrate. CI is in unique position to echo how the work of IUPAC and the evolution of the PT crisscrossed. Following this idea, the January 2019 issue was conceived, reviewing how IUPAC contributes to the curation of the information presented in the Periodic Table. This short article is an invitation to look forward to the January 2019 CI issue, and also to forth coming issues in 2019 which will (re) connect you with IUPAC. (See *CI* Jan 2019 contents at https://iupac.org/etoc-alert-chemistry-international-jan-mar-2019/). The January issue introduction is co-signed by Jan Reedijk and Natalia Tarasova; together they co-chair the Management Committee coordinating IYPT.

The history of the Table itself and how scientists came to organize the elements is well studied and these events predated IUPAC. A glance of that history is presented by G.J. Leigh in the feature titled "IUPAC and the Periodic Table" (*CI* Jan 2019, p. 6). When IUPAC became involved clearly illustrates how the Union can contribute toward *Creating a Common Language for Chemistry*. That very theme of *Creating a Common Language for Chemistry* is the motto of the IUPAC centenary celebration (more about that below). For example, Leigh explained briefly how till mid 80s there were numerous confusions in the literature related to the different designation of Group (vertical column in the table) for the same group of elements, such as IVA and IVB, employed on opposite sides of the Atlantic. To make sense of the literature of the time, the reader had to remember where the writer of the article was based. And "to sweep aside the international confusion, the human overseers of the kingdom formed a kind of United Nations to agree on the nomenclature they would use." These last words are quoted from Peter W. Atkins who in his book titled "The Periodic Kingdom" spoke of the Table as the *Land of the Chemical Elements*, reviewing the geography, the history, and the institutions by which it is governed[1]. The "kind of United Nations" he referred to is the International Union of Pure and Applied Chemistry.

Leigh also describes how a naming system for elements yet to be discovered was developed, how the Union has established a protocol to review and to assess the discovery of new elements, and how new elements get their name. As a long-time member of IUPAC and former President of the Inorganic Chemistry Division, Leigh also recounts anecdotes. Being the first in the issue, his feature provides context for those that follow.

A Field of Allure and Romance is a fascinating account prepared by Sigurd Hofmann who, reviews in some details how the criteria of new element discovery were set and again recently reviewed (*CI* Jan 2019, p. 10). Such an account is timely because not only it recalls the original 1991's work of the joint IUPAC-IUPAP Transfermium Working Group, it also provides an update about the contemporary work again coordinated jointly with IUPAP and more recently published in November 2018[2].

Hofmann quotes excerpts of the original 1991 TWG report which provides exciting insight on the spirit behind the study of new elements. The following excerpt echoes the mysterious attraction:

"The centuries-old history of the definition and discovery of chemical elements has a deep scientific and general fascination. This is because the problem is of an

essentially finite scope: there can only be a limited number of species of atomic nuclei containing different numbers of protons that can be imagined to have an existence, though perhaps only fleeting, in the chemical sense. But although the problem is of finite scope, we do not know what the scope is: we do not as yet know how many elements await discovery before the disruptive Coulomb force finally overcomes the nuclear attraction. In this sense, the problem is open although of finite scope, unlike the number of continents upon the surface of the earth where we know with certainty that none still awaits discovery. These considerations give to the discovery of new elements an importance, an allure and a romance that does not attach to the discovery of, say, a new comet or a new beetle where many more such discoveries are to be anticipated in the future."

Hofmann reviewed the context of the original work and how it has evolved since. The exploration remains ever challenging, and ultimately, Hofmann's account shows how rules and criteria prevail and how they complement and facilitate communication.

There is also in that CI feature another quirky reference to allure: a unique photo of the TWG group back in June 1989 meeting in Berkeley. The photo shows the nine members of the TWG and Glenn Seaborg as the host of the group. With allure no less, Professor Seaborg wore an IUPAC tie! (CI editor thanks Robert Barber who resurfaced and shared this photo.)

The Periodic Table is today a communication and education tool. Its elaboration was a process and as history tells us, it started for Mendeleev as an attempt to devise an ordering system that will make sense for his students and to illustrate his 1869 introductory textbook "Principles of Chemistry". In a concise feature (*CI* Jan 2019, p. 16), Eric Scerri provides an account of the development of the Table. From the short form with eight columns to medium long with 18, or even longer with 32 columns, Scerri explains how and why the Table still shows variances in the way it is portrayed today.

With the Table finally set to order elements by atomic numbers, chemists came to use the Table to report atomic weights. The reported values of atomic weights -*i.e.* relative atomic masses- have evolved and continue to evolve due to better instrumentations and improved analytical techniques. Still today, the values are regularly and critically reviewed, and a committee/commission is entrusted with the task of publishing updates. A two-part account of the work of the Commission on Isotopic Abundances and Atomic Weights (CIAAW) and its preceding body, is published (*CI* Jan 2019, p. 21). Part one, originally prepared by John DeLaeter in 1999, provides a historical account CIAAW and how it constitutes a critical service to Chemistry and its development, progress, and application. In part two, Juris Meija, current chair of CIAAW, shares a portrait of CIAAW and explains how it remains to be relevant for the community till this day.

The relevance that *Isotopes Matter* is the subject of another article co-authored by Norman Hoden, Tyler Coplen, and Peter Mahaffy (*CI* Jan 2019, p. 27). That feature is also timed with the recent release in December 2018 of a detailed element-by-element review[3]. That review accompanies a Periodic Table of the Elements and Isotopes created to familiarize students, teachers, and non-professionals with the existence and importance of isotopes of the chemical elements. In addition to providing the chemical name, symbol, atomic number, and standard atomic weight of an element, that Table is color-coded and provides pie charts displaying for each element the isotopes entering in the determination of the standard atomic weight. This work is ultimately the support behind a website bearing the same name isotopesmatter.com developed by the King's Center for Visualization in Science (King's University, Edmonton, Canada) and that sprung from a IUPAC project also involving the Committee on Chemistry Education. The review provides multiple examples of practical applications of isotopic measurements and technologies, including in the fields of forensic science, geochronology, Earth-system sciences, environmental science, and human health sciences.

One last timely feature published in the January 2019 CI is co-authored by Ian Mills and Roberto Marquardt about the new International System of Units (SI) (*CI* Jan 2019, p. 32). Approved last November, the new SI will come into force on 20 May 2019. The new SI now includes seven defining constants and this brings to an end the

use of physical artefacts to define measurement units. The change follows that of the recent redefinition of the mole which IUPAC completed only a few months prior[4]. The new SI does not directly relate to the Periodic Table, but the timing of its release and of its implementation timed for May 2019 can not escape the celebratory spirit of the year 2019 (see also the article by Brynn Hibbert in this CITAC News issue, p. 61).

Later this year, another issue of *Chemistry International* will focus on IUPAC history. In a recent editorial, IUPAC President Qifeng Zhou recalled IUPAC earlier years and framed concisely the Union's role in *Creating a Common Language for Chemistry*: "Established in 1919, in the aftermath of the First World War, IUPAC nurtured a scientific community eager to reengage constructively in international exchanges. To support such endeavor, communication was paramount, both to ensure unambiguous sharing of scientific information for the support of research and to facilitate trade and commercial activity. The chemists who established IUPAC saw the needs to create a nomenclature that would facilitate communication in chemistry in the broad sense, developing universally-accepted terminology and nomenclature. Today, that mandate broadens as research expands, for example in new materials. Communication also has new requirements and the human language is no longer the only one required for scientific exchanges. Today, global research also involves sharing information digitally, and providing ways through which computers can 'talk chemistry' is a challenge which IUPAC is currently addressing.[5]"

Aside from the Fennell and Brown's History of IUPAC book set 1919-1987[6], there are few accounts of IUPAC history. The centennial provides the incentive for a group of historians, archivists, and researchers to devote time exploring IUPAC old records. Their findings will be shared during a special symposium held during the 2019 IUPAC Congress to be held in Paris early July. This shall be a very interesting session, as again reminded by Zhou quoting a Chinese proverb (5) "If you want to learn about the future, you have to look into the past".

Between IYPT and IUPAC100, there will be in 2019 numerous occasions to celebrate. A partial list of events and on-going activities is provided as an incentive to participated and get engaged; see more details and more at iypt.org and iupac.org/100/. Invited to find *my* element, I have retrieved my 'Fm' pin which I will wear in 2019 with fun and *allure*. Fermium is afterall element 100 and that provides a quirky coincidence at the intersection of IYPT and IUPAC100!

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2. S. Hofmann, *et al.* (2018). On the discovery of new elements (IUPAC/IUPAP Provisional Report), *Pure Appl. Chem.* 90(11), pp. 1773-1832.
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SELECTION OF INTERNATIONAL ACTIVITIES TO CELEBRATE IYPT2019 AND IUPAC 100

Dates	Activity Description	Website
July 2018 - July 2019	IYCN/IUPAC100 Periodic Table of Younger Chemists	https://iupac.org/100/pt-of-chemist/
Jan 8 – Dec 31	IUPAC Periodic Table Challenge	https://iupac.org/100/pt-challenge/
January 29	Official IYPT Opening at UNESCO	www.iypt2019.org
Jan 31	Chemistry Rediscovered - EYCN Video contest deadline	https://www.euchems.eu/divisions/european-young-chemists-network/chemistry-rediscovered/
Feb 8	IYPT Opening ceremony in Russia on Mendeleev birthday	
Feb 11-12	Murcia Symposium: Setting their Table: Women and the Periodic Table of Elements	http://www.iypt2019women.es/scientific_topics.php
Feb 12	Empowering Women in Chemistry: A Global virtual Networking Event	https://iupac.org/100/global-breakfast/
Mar 31	IUPAC's Role in Creating a Common Language for Chemistry	https://iupac.org/event/iupacs-role-in-creating-a-common-language-for-chemistry/
12-19 May	IUPAC for Africa – Postgraduate summer school on Green Chemistry	https://iupac.org/event/iupac-for-africa-postgraduate-summer-school-on-green-chemistry/
May 20	World Metrology Day to coincide with the implementation of the new SI	
July 5-12	IUPAC Congress and General Assembly, Paris, France	www.iupac2019.org
July 26-28	Mendeleev 150 – 4th International Conference on the Periodic Table	https://mendeleev150.ifmo.ru/
July 28	IUPAC 100th birthday!	
July 21-30	51st International Chemistry Olympiads, Paris, France	https://icho2019.paris/
December 5	Official IYPT Closing ceremony, Tokyo, Japan, hosted by Science Council of Japan IUPAC subcommittee	http://www.iypt2019.jp/eng/index.html

TALANTA: ITS BEGINNING AND EVOLUTION

Dedicated to the IUPAC 100 years celebration, with congratulations from the Talanta team

Gary D. Christian // University of Washington, USA
Jean-Michel Kauffmann // Université Libre de Bruxelles, Belgium
Co-editors-in-chief, Talanta

Talanta, the International Journal of Pure and Applied Analytical Chemistry, originated in 1958, at the recommendation of Professor Ronald Belcher (Figure 1) of the University of Birmingham in England (1, 2). He had become disenchanted with the standards of some analytical journals and by chance met with Robert Maxwell who owned Pergamon Press, Ltd. and wanted to expand his repertoire of scientific journals. And a deal was struck. Maxwell bought Pergamon Press , Ltd. from Springer Verlag in 1951, and sold it to Elsevier Science, Ltd. In 1991.

Figure 1: Professor Ronald Belcher, University of Birmingham, England initiated the founding of Talanta

Figure 2: Professor Cecil Wilson, Queens University Belfast, the first editor of Talanta

EDITOR HISTORY

Professor Cecil Wilson (Figure 2) of Queens University Belfast was the first editor. The first issue was published in August, 1958 (Figure 3). Manuscripts were accepted in English, German, and French, and abstracts were published in all three languages. This policy remained for thirty years. The forward for the first issue was written by Fritz Feigl, stating "Existing journals are not sufficient to ensure the rapid publication which is demanded both by authors and readers. It is therefore opportune that TALANTA, this new international journal of analytical chemistry in its broadest sense, is being introduced."

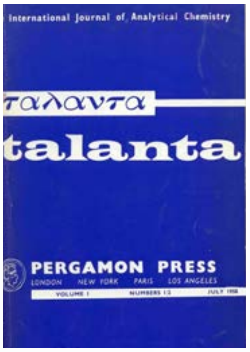

Figure 3: 1st issue of Talanta, published 8/1958.

The first paper was a review by F. E. Beamish of the University of Toronto, "A critical evaluation of the gravimetric methods for the determination of platinum metals". Other initial contributions included research papers from luminaries E. H. Swift, H. Flaschka, H. Diehl, C. N. Reilley, R. Přibil, R. Belcher, and T. S. West, in addition to Feigl.

The symbol for the journal is a Greek balance taken from one of the Hope Vases (Figure 4). The name Talanta derives from the Greek word ταλαντα, used by Homer to mean "a pair of scales(3). It is related to the Greek "talent", a weight of gold or silver, and such balances were used for measurements of talents, or gold coins.

Figure 4: The symbol for the journal is Greek balance taken from one of the Hope vases.

Cecil Wilson remained editor until his retirement in 1965. Maurice (Mo) Williams served a short time until he was appointed managing editor at Pergamon. Then Robert A. Chalmers (Figure 5) from the University of Aberdeen, Scotland was appointed Editor-in-Chief in January, 1966, and remained 23 years until his retirement at the end of 1988. Bob was incremental

Figure 5: Robert A. Chalmers was appointed ad Editor-in-Chief in 1966, and remained for 23 years

in furthering the journal, checking experiments in the laboratory, doing detailed copy editing, and assuring high quality publications. His remarkable contributions are chronicled in an obituary by his colleague Mary Masson (4).

Figure 6: Gary Christian was appointed joint-editor-in-chief in 1989, serving to this date

Figure 7: David Littlejohn was appointed joint-editor-in-chief in 1989, and served till 1991

In 1989, Gary Christian (Figure 6), University of Washington, USA, and David Littlejohn (Figure 7), University of Strathclyde, Scotland, were appointed as Joint-Editors-in-Chief. At that time, manuscript assignments were apportioned to the editors by geography, and this remains to date. Also, beginning then, manuscripts were accepted only in English.

Figure 8: Elo Hansen was appointed as joint-editor-in-chief in 1991, serving until 1995

Figure 9: Jean-Michel Kauffmann was appointed co-editor-in-chief in 1995 serving to this date

David resigned in 1991, and Elo Hansen (Figure 8), Technical University of Denmark, replaced him, serving until 1995. At that time, Jean-Michel Kauffmann (Figure 9), Université de Bruxelles, was appointed as co-editor-in-chief, and remains today.

As manuscript flow increased, Associate Editors were added to help with manuscript editing, appointed by geography.

Figure 10: James Winefordner served as Chairman of the Editorial Board from 1984 to 2005

James D. Winefordner (Figure 10), University of Florida, USA served as Chairman of the Editorial Board from 1984 to 2005, a period of 21 years, and was critical in advising and maintaining high standards for the journal. A tribute to his contributions was detailed in an editorial (5).

JOURNAL FOCUS

Talanta's Guide for Authors (6) details our current aims and scope and types of papers. Full papers, short communications, and rapid communications are accepted. The criteria for manuscripts are listed as follows: Analytical performance of methods should be determined, including interference and matrix effects, and methods should be **validated** by comparison with a standard method, or analysis of a certified reference material. Simple spiking recoveries may not be sufficient. The developed method should especially comprise information on selectivity, sensitivity, detection limits, accuracy, and reliability. *However, applying official validation or robustness studies to a routine method or technique does not necessarily constitute novelty.* Proper statistical treatment of the data should be provided. Relevant literature should be cited, including related publications by the authors, and authors should discuss how their proposed methodology compares with previously reported methods.

JOURNAL STATISTICS

The impact factor for Talanta is currently 4.244. Time for editorial review and author revision is about 4.5 weeks, and within less than a week the first version of the article is visible online to the readers.

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CITAC
Cooperation on International Traceability in Analytical Chemistry

CHANGING THE WORLD OF METROLOGY IN CHEMISTRY

THE NEW MOLE IN THE NEW INTERNATIONAL SYSTEM OF UNITS (SI)

D. Brynn Hibbert // UNSW, Sydney, Australia, Secretary of ICTNS of IUPAC

In April 2018 the CITAC Vice-Chair Bernd Güttler wrote an address summarizing the changes to the definition of the mole and giving a brief history of the discussions that have gone on since the 1970s[1]. He is in an excellent position to tell us about the new mole, being Chair of the "CCQM *ad hoc* Working Group on the Mole[2]". As I write this article the group has published a draft *mise-en-practice*[3].

But first I return to just over a month ago waiting for the news that the CGPM had agreed unanimously to the 'New SI'. As a sign of our modern age on 16 November 2018 in Sydney I could watch the You Tube video of the Australian delegate casting his vote in favour of the changes to the SI at the 26th meeting of the General Conference on Weights and Measures (CGPM) in Versailles, France[4].

The mole is now (or will be on 20th May 2019) defined:

> 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 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.

IUPAC, or at least its Analytical Division, first heard of the proposed changes at its Glasgow General Assembly in 2009 from that doyen of metrology Ian Mills. Then the proposed changes were not exactly what have been approved in the 2018 vote, but they did involve fixing the value of N_A, and were supported by the Council of IUPAC with the caveats:

1. The greatest effort should be made to change the name of the ISQ base quantity "amount of substance" at the same time that a new definition of the mole is approved.
2. A note should accompany the new definition to explain that the molar mass of ^{12}C will be an experimental quantity, with a relative measurement uncertainty of about 1.4 × 10^{-9}.

1 http://www.citac.cc/CITAC_News_2018_WEB.pdf, pages 4, 5
2 https://www.bipm.org/en/committees/cc/wg/mole.html
3 https://www.bipm.org/cc/CCQM/Allowed/22/CCQM16-04_Mole_m_en_p_draft_2018.pdf
4 https://www.youtube.com/thebipm

In the following decade there was a movement within IUPAC to reassess the support. We were not so happy that the unit of mass would not be defined by an object that actually had mass (chemists tended to support systems based on the atomic mass unit or dalton). However it must be said that it was the nature of the quantity 'amount of substance' that caused most problems. The CIAAW (Commission on Isotope Abundances and Atomic Weights), although a commission of IUPAC, was very active in challenging the proposed new definition. In 2011 in a special edition of ACQUAL[5] the different arguments were rehearsed. IUPAC reacted very well to internal and external disquiet by establishing an interdivisional project to review its stance on the proposed redefinition of the mole (and kilogram)[6]. Its National Adhering Organisations (NAOs) were invited to comment and on the whole were prepared to live with the new definitions. The project report[7] offers essentially the definition that was finally adopted by the CCU, but did not suggest any changes to the quantity amount of substance. The late Paul De Bièvre visited the issue in a number of his editorials in ACQUAL summing up in 2014 with an article titled "CCQM owes chemists a description of the concept 'amount of substance'" [8].

AMOUNT OF WHAT?

What is wrong with amount-of-substance as a continuous variable and kind of quantity for which the mole is a unit? It must be said that chemists have long been comfortable with counting entities and understand that atoms are discrete. The principles of stoichiometry make us at home with a concept in which atoms or molecules react in whole number proportions, and simply taking a suitably large number of these entities, sufficiently large enough to easily weigh, works for us. Thus the idea of the gram molecule (aka mole) makes intuitive sense and does not require a quantity to attach it to. The modern SI gave us amount-of-substance in 1971 (as the BIPM site says "after lengthy discussions between physicists and chemists"). Bernd Güttler explains that in 1971 it was taken for granted that measurements at the atomic scale, for example visualising or counting atoms, were impossible and would always be impossible. By 2019 he quotes the IUPAC project: "With the recent advances in science and measurement practice, our ability to determine the value of the Avogadro constant has now reached a level of relative uncertainty that allows a redefinition of the mole in terms of the explicit number of elementary entities. ... it realigns the definition of the mole with the way most chemists understand it."

This is true, and so have we outgrown amount of substance? One of the architects of the 1971 definition of the mole as part of the SI, Max McGlashan, wrote to Paul De Bièvre in 1996 "... if any change were needed [to accommodate a new mole as a mass or a number] then abandoning amount of substance altogether would be much less unattractive. Though widely used by chemists, the physical quantity called amount of substance and its SI unit called the mole are not necessary in science" [quoted in [8]].

At a meeting of the CCQM in 2014 I gave a paper on the redefinition of the mole in which I reviewed first year undergraduate chemistry textbooks written in English (admittedly an *ad hoc* collection of current texts that I could find in my University Library). The results were astounding (See Table 1 below). Chemists had not embraced amount of substance but continued to use the concept of a countable number of entities, defining a mole almost invariably as "an Avogadro number of entities", and speaking as if the relevant quantity were "number of moles". It is interesting that no writer of a text book could simply copy out the definition of the mole from the SI Brochure. They must have known about the SI but presumably decided it was not helpful in their chemistry courses to reproduce an accurate definition. We who are steeped in metrology should take note that while what we say is often 'law', especially when backed by the CGPM or IUPAC General Assembly, it does not mean

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5 Accred Qual Assur (2011) The re-definition of the mole must be of high quality, 16:117-174, March 2011

6 Stohner, J.; Marquardt, R.; Meija, J.; Mester, Z.; Towns, M.; Weir, R., A Critical Review of the Proposed Definitions of Fundamental Chemical Quantities and their Impact on Chemical Communities. *IUPAC Project 2013-048-1-100*, **2013**.

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

8 De Bièvre, P., CCQM owes chemists a description of the concept 'amount of substance'. *Accred. Qual. Assur.* **2014,** *19* (4), 323-325.

that our community will slavishly follow our diktats.

I have no reason to believe the situation has changed in 2019, although perhaps the focus on the New SI might cause some reassessment, and acknowledgement that the SI is now more in keeping with the chemists' view of the world.

Table 1: Review of the mole concept and amount of substance in first year university chemistry text books (Hibbert 2014)

Concept	Number / total texts
"Amount of substance" in index	3/18
"Amount of substance" referred to in text correctly	4/18
N_A correctly identified as the Avogadro constant with unit mol^{-1}	4/18
Correct SI definition of mole	0/18
Explicit analogy of N_A with dozen (usually called Avogadro number)	10/18

In returning the Avogadro number to the SI (note: there is no mention of the 'Avogadro number' in the 1971 definition of the mole, or indeed anywhere in the SI Brochure[9]), the New SI legitimises the chemists view of the mole.

REALISING THE MOLE

The CCQM working party have noted that, at present, the most accurate realization of a mole[10] involves the measurement of the number of ^{28}Si atoms (N) in a single crystal of Si, enriched in ^{28}Si, using volumetric and X-ray interferometric measurements, the output of the so-called 'Avogadro project'. This experiment was carried out within the framework of the International Avogadro Coordination and was fundamental to determining the best experimental values of both the Avogadro and Planck constants prior to fixing their values. The amount of ^{28}Si, $n(^{28}Si)$, in a crystal of volume V_s is:

$$n(^{28}Si) = 8V_s/(a(^{28}Si)^3N_A)$$

where $a(^{28}Si)$ is the lattice parameter of the cubic cell of ^{28}Si containing 8 atoms of ^{28}Si, and N_A is the Avogadro constant, giving the unit mol to n.

Of course, this experiment was useful when establishing a numerical value for the Avogadro constant, but is not a practical route to the amount of substance of the majority of chemicals.

The working party give three practical realisations of the mole: gravimetric preparation, use of the ideal gas law, and electrolysis. For example the amount of substance transformed by the passage of Q coulomb of electricity is

$$n = Q/(zeN_A)$$

where z is the charge number of the reaction and e is the electronic charge (exactly $1.602\ 176\ 634 \times 10^{-19}$ C in the New SI). Note that because the Avogadro constant and the electronic charge are both fixed, the numerical value of the Faraday constant = eN_A will now also be fixed.

For chemists the most used measurement of amount of substance is via mass and a knowledge of the molar mass, i.e. by weighing a pure substance, or measuring a mass concentration or mass fraction of a solution or mixture. Consider a sample of a material mass m containing a mass fraction $w(X)$ of substance X. Then

$$n(X) = w(X)m/(A_r(X)N_Am_u)$$

where $A_r(X)$ is the relative atomic or molecular mass of X and m_u is the atomic mass constant ($N_Am_u = M_u$, the molar mass constant). The atomic mass constant m_u is 1/12 of the mass of a free ^{12}C atom, at rest and in its ground state, and is an experimentally-determined quantity. An advantage of the new definition is that macroscopic (e.g. n and M_u) and microscopic (e.g. N and m_u) quantities

[9] BIPM *The International System of Units (SI) Updated 8th Edition*; Intergovernmental Organisation of the Convention of the Metre: Sevres, France, 2014. https://www.bipm.org/utils/common/pdf/si_brochure_8.pdf

[10] I use 'a mole' rather than 'the mole' as the realisation depends so much on the nature of the entities.

have the same relative uncertainties because they are related through N_A which has no uncertainty.

CONCLUSION

So on May 20th 2019, International Metrology Day, let us toast the New SI, and particular the new, countable, mole, and perhaps no longer worry quite so much about amount of substance.

The first steps of a new forum in Portuguese:

FORMEQ - INTERNATIONAL FORUM ON METROLOGY AND EXAMINOLOGY IN CHEMISTRY

Ricardo Bettencourt da Silva
Tony Dadamos

Portuguese is the sixth most natively spoken language in the world and the most spoken language in the Southern Hemisphere. The 220 million native speakers of Portuguese have, together with the language, many other affinities grounded on centuries of multicultural relations. Fernando Pessoa, a famous poet, stated that "*My nation is the Portuguese language*" making a citizen of a small country a member of a large community. The 'Community of Portuguese Language Countries' (CPLP) is particularly active in promoting the collaboration between members of this huge community.

In this global world – for some an invention of the Portuguese discoveries – we also share the problems and face the same challenges of many other communities. One of those, is the comparability and quality of measurement and examinations in chemistry.

Having in mind the similarity of problems faced in different latitudes using a common language, some Brazilian and Portuguese chemists, from private and public organisations, decided to join efforts in promoting the quality of characterisations in chemistry in Portuguese spoken countries. ForMEQ, International Forum on Metrology and Examinology in Chemistry, will join citizens of CPLP countries in discussing this issue while engaged to collaborate with national organisations that act in this area. ForMEQ has also the particularity of encouraging individual membership that allows the participation in this project of people with various backgrounds and experience with a common motivation: to make sure chemical characterisations will play their role properly.

ForMEQ has 41 founding members from Brazil and Portugal but will attract the active participation of chemists from other Portuguese speaking countries.

The general and specific objectives of ForMEQ are the following ones:

GENERAL OBJECTIVES

ForMEQ intends to endorse the international cooperation between Portuguese Speaking Countries in the promotion of the quality of measurements and examinations in chemistry. This Forum has started from a Luso-Brazilian cooperation in this area but aims to extend their geographical distribution. It promotes working groups, conferences and training actions in the field of quality and metrology and examinology in chemistry (the sciences of quantitative and qualitative analysis in chemistry, respectively), taking into account the needs and priorities of the community.

SPECIFIC OBJECTIVES

- To encourage the culture of quality assurance;
- To promote events (forums, conferences, workshops and training courses) on metrology and examinology in chemistry;
- To put forward the development of guides and tutorials on metrology and examinology in chemistry;
- To disseminate good laboratory practices in the production and interpretation of measurements and examinations in chemistry;
- To contribute to the elimination of artificial trade barriers resulting from the failure to correctly obtain and interpret measurement and examination results.

We wish ForMEQ will fulfil the ambitious expectation of their members by giving them the opportunity to collaborate in promoting the quality of chemical characterisations in Portuguese.

JOINING THE METRE CONVENTION BY UKRAINE AND UKRAINIAN ACTIVITIES IN METROLOGY IN CHEMISTRY

Mykhailo Rozhnov, Ovsiy Levbarg // Ukrmetrteststandart, Ukraine

JOINING THE CONVENTION

On May 23, 2018 the Ukrainian parliament, Verkhovna Rada, has approved its shortest probably law, which is concise enough to reproduce it in full: "Verkhovna Rada of Ukraine decrees: to join the Metre Convention concluded on May 20, 1875 in the city of Paris (the Convention is attached)". Although the mass media paid not so much attention to this news, it was appreciated by the metrological community and all those who were aware of importance of being integrated into the global measurement system.

Joining the Metre Convention has been an important step in course of development of the Ukrainian system of technical regulation required by the Ukraine–European Union Association Agreement. Joining the Convention was preceded by adoption of the updated legislation: Law on Metrology and Metrological Activities, Law on Standardisation, and Law on Technical Regulations and Conformity Assessment.

These developments influence also the progress in metrology in chemistry. The institution responsible for this metrology field in Ukraine is Ukrmetrteststandart.

UKRMETRTESTSTANDART

Ukrmetrteststandart is a hardly pronounceable abbreviation for the Pan-Ukrainian Research and Production Centre for Standardisation, Metrology, Certification, and Consumers' Protection. Its history goes back to 1902, when, by initiative of D.I. Mendeleev, a Verification Chamber of Measures and Weights was established in Kiev. By now, as its full name says, Ukrmetrteststandart is a multitask organisation, and all its functions are associated with metrology.

Our activities in metrology in chemistry have originated from measurements of the thermodynamic properties of gas mixtures and gas analysis of late 1960's and early 1970's. In the former USSR we shared the responsibility for gas analysis metrology with the D. I. Mendeleev Institute of Metrology in Leningrad (now St. Petersburg) and maintained the reference gas composition standard for the southern area of the USSR. After Ukraine had

gained independence, this standard has been upgraded to the National Primary Standard of Ukraine.

PRIMARY AND REFERENCE MEASUREMENT STANDARDS

Ukrmetrteststandart has been charged with establishing national standards in the field of metrology in chemistry. The first one was the mentioned National Primary Standard for the gas mixtures composition. It comprises high-accuracy equipment for preparing and analysing gas mixtures and a set of gravimetrically prepared primary standard gas mixtures. To remain state-of-the-art, the National Primary Standard is permanently renovated.

Later on two National Primary Standards of electrochemical quantities have been established: the National Primary Standard of electrolytic conductivity and the National Primary Standard of pH. Similarly to the gas composition standard, they consist of the measurement systems (the main parts are conductometric cells – for electrolytic conductivity, coulometric titrator and electrochemical cells – for pH), sets of the standard solutions and equipment for their preparation. Major parts of the standards were designed and produced by Ukrmetrteststandart and other Ukrainian companies.

Ukrmetrteststandart maintains also primary and reference measurement standards for quantities of adjacent metrology fields: humidity, viscosity, density, as well as optical quantities.

The National Primary Standard of gas humidity is mostly aimed to meeting natural gas industry demands for metrological traceability of water content measurements. It comprises generators realising the values of gas relative humidity, dew point and water mole fraction.

The National Primary Standard of the refraction index of liquids and solids in the visible part of spectrum comprises primary standard prisms, primary standard liquids, and complex of technical means to realise the values of the refraction index.

Our reference standards of liquids viscosity and liquids density are being upgraded now to become the next National Primary Standards.

Whatever perfect the national measurements standards may be, they are of limited value until they are not recognised internationally. The main way to get the international recognition is to take part in the international comparisons and to have calibration and measurement capabilities (CMCs) published afterwards.

INTERNATIONAL COMPARISONS AND CMC$_s$

Our measurements standards have taken part in a number of the international key and supplementary comparisons, organised by the regional metrology organisations, COOMET mostly, but also by the Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology (CCQM) directly. By now, most of the comparisons, we have taken part in, belonged to the gas analysis area. To mention the recently finished ones, those were COOMET.QM- K93 "Ethanol in nitrogen", COOMET.QM-K111 "Propane in nitrogen", and COOMET.QM-S5 "Carbon monoxide, carbon dioxide, propane in nitrogen ("automotive" gas mixtures)". The National Primary Standards of electrochemical quantities have also successfully participated in the inter-comparisons in the electrolytic conductivity and pH fields, e.g. CCQM-K18, CCQM-K36, CCQM-K105, COOMET.QM-K36, etc. We have taken part also in the comparisons related to some other areas of interest, e.g. CCQM-K130 "Nitrogen mass fraction measurements in glycine", SIM.QM-K27 "Ethanol in Aqueous Matrix", COOMET.PR-S3 "Refractive Index", COOMET.M.V-K1 "Liquid viscosity measurements".

Successful participation in the inter-comparisons, in conjunction with the results of the peer-reviews of our institution by COOMET, made it possible for us to have CMCs published in the BIPM key comparison database. Currently our published CMCs in chemical analytical and associated measurements relate to gas analysis, including all the important categories of gas mixtures (environmental, fuel, forensic, high purity gases), electrochemical quantities, high purity chemicals, kinematic viscosity.

It is worth mentioning that the CMC tables concerning CCQM-related quantities contain two major parts, with distinct measurand ranges and uncertainties (that may coincide, but not necessarily): one for measurement

capabilities and another one for the certified values of the produced reference materials.

REFERENCE MATERIALS

Reference materials (RMs) are the key tools for establishing metrological traceability in analytical measurements, and important at all the levels of calibration chains, including the highest ones. Thus, we produce RMs both for maintaining our primary measurement standards mentioned above and also to serve the needs of our customers. Some of the RMs are covered with the published CMCs, e.g. calibration gas mixtures, pH buffer solutions, electrolytic conductivity CRMs. We also produce other RMs, including those for moisture and protein content in grain and grain products, sulphur in oil products, density and viscosity of liquids, refraction index etc. There are also other RM producers in Ukraine. With regard to RMs production, our quality management system has been certified according to ISO Guide 34, and now we are preparing for the certification vs. ISO 17034. It presumes practical adoption of the recent versions of ISO/REMCO Guides on reference materials.

In general, ISO standards and guides, as well as Eurachem and Eurachem/CITAC documents, are very essential to all our work.

ISO & EURACHEM

We use widely the international documents. For example, ISO standards on the calibration gas mixtures preparation and analysis are the normative basis for our National Primary Standard of gas composition. At the same time, we go beyond merely using the standards. For many years our representatives have contributed to development of the international standards at the ISO/TC 158 - Analysis of Gases, and ISO/TC 193 - Natural Gas. This started as far back as 1980's, when Dr. Rozhnov became a chair of the "permanent Soviet part" at the ISO/TC 158. This technical committee deals with the standards related mostly to metrological traceability of gas composition measurements, i.e. methods for preparing and analysing calibration gas mixtures, impurity analysis, general aspects of metrological traceability. Some of those standards, e.g. ISO 6143 and ISO 12963 providing calibration methods or ISO 19229 setting requirements for the purity analysis, may be applied not just to gas analysis, but also for other chemical analytical tasks.

As to the standards under the responsibility the ISO/TC 193, to a great extent they deal with analytical methods applied in the specific field of natural gas analysis, which is highly important for Ukraine. ISO 6974 series of standards on gas chromatography analysis should be mentioned in this context, and again, the approaches stated in these documents with regard to calibration and measurement uncertainty evaluation may be useful beyond the natural gas field. We take part also in the committee's working groups dealing with the calculation of the natural gas properties, which has been our area of interest for a long time.

In addition, our representative has become recently a committee member at the ISO/REMCO.

Another area of our international activities is Eurachem. A decision on admitting Ukraine to Eurachem has been taken in 2000, and one year later the Memorandum of Understanding was signed on behalf of Ukraine at the Eurachem General Assembly in Popowo, near Warsaw. Since then we have been working together with Eurachem colleagues, and now we have our representative in the Measurement Uncertainty and Traceability working group.

Another side of our international work is translating the documents to adopt them in Ukraine.

TRANSLATIONS AND TERMINOLOGY

We have translated into Ukrainian about forty ISO standards on gas analysis and natural gas, three Eurachem guides: Terminology in Analytical Measurement. Introduction to VIM 3 – into Ukrainian; The Fitness for Purpose of Analytical Methods. A Laboratory Guide to Method Validation and Related Topics – into Ukrainian and Russian; Measurement Uncertainty Arising from Sampling: a Guide to Methods and Approaches – into Russian; and five Eurachem leaflets, all into Ukrainian. All the Ukrainian translations may be downloaded directly from the Eurachem website, and Russian translations are available on request, also free of charge. Besides

ISO and Eurachem documents, we have also translated (into Russian) the IUPAC Technical Report "Metrological traceability of measurement results in chemistry: Concepts and implementation".

While translating, we occasionally encounter some problems with terminology. Generally, the Ukrainian terminology for science and technology does exist, but the difficulties arise mostly due to two reasons: first, after the period of an intensive elaboration in the 1920's, development of the Ukrainian terminology was retarded, and until recent times the Russian language has been prevailing; as a result, some gaps and discrepancies in the Ukrainian terminology appeared, and it is also our work to fix them; second, continuous progress in science, including metrology, calls for new terms or redefinition of the old ones and respective adoption of the novelties into national languages. So, the problems with the terminology take place both on national and global levels, and it is clearly evidenced by the continuous work on the consecutive versions of the VIM. Belonging to the metrological community, we hope to contribute to harmonisation of the global terminology in metrology, especially in chemical analysis and associated areas. And it is just a part of our prospects.

OUR PROSPECTS

With regard to joining the Metre Convention, we have to benefit as much as possible from this attainment, first of all, by joining the CCQM and its working groups. It will give us more possibilities for the international recognition of our measurement standards and development of the metrological system in the country. Of course, we are going to continue our work with the ISO technical committees closely linked to metrology in chemistry, and with Eurachem. Certainly, we'll do our best to contribute properly to the international activities, still with the great help from our friends.

ACKNOWLEDGMENTS

To conclude, let us express our hearty gratitude to all our teammates in Ukraine we have been working together with for many years and hope to carry on, as well as to the colleagues from all around the globe whose permanent support and assistance we do appreciate.

PROFESSOR DMITRI MENDELEEV – A CHEMIST, A METROLOGIST, A TEACHER AND AN INDUSTRIALIST

Yu. A. Karpov // Association of Analytical Centers "Analitica", Russia
V. Baranovskaya // GIREDMET, Russia

The United Nations has declared 2019 as the International Year of the Periodic Table of Chemical Elements (IYPT 2019) to celebrate the 150th anniversary of the periodic table established by Dmitri Mendeleev, and to promote its significance and applications to society.

The distinguished Russian chemist Dmitri Mendeleev has created his first diagram of the Periodic Table in 1869 and sent a scientific notice about this crucial discovery to the world leading chemists of that time.

According to his Periodic Law all properties of chemical elements are changing as their atomic weight increases, so similar elements or the elements with nearly identical properties appear in the defined intervals of the atomic weights. Mendeleev was not only one who has accurately formulated this law and presented its content in the form of the table which has become classic, but

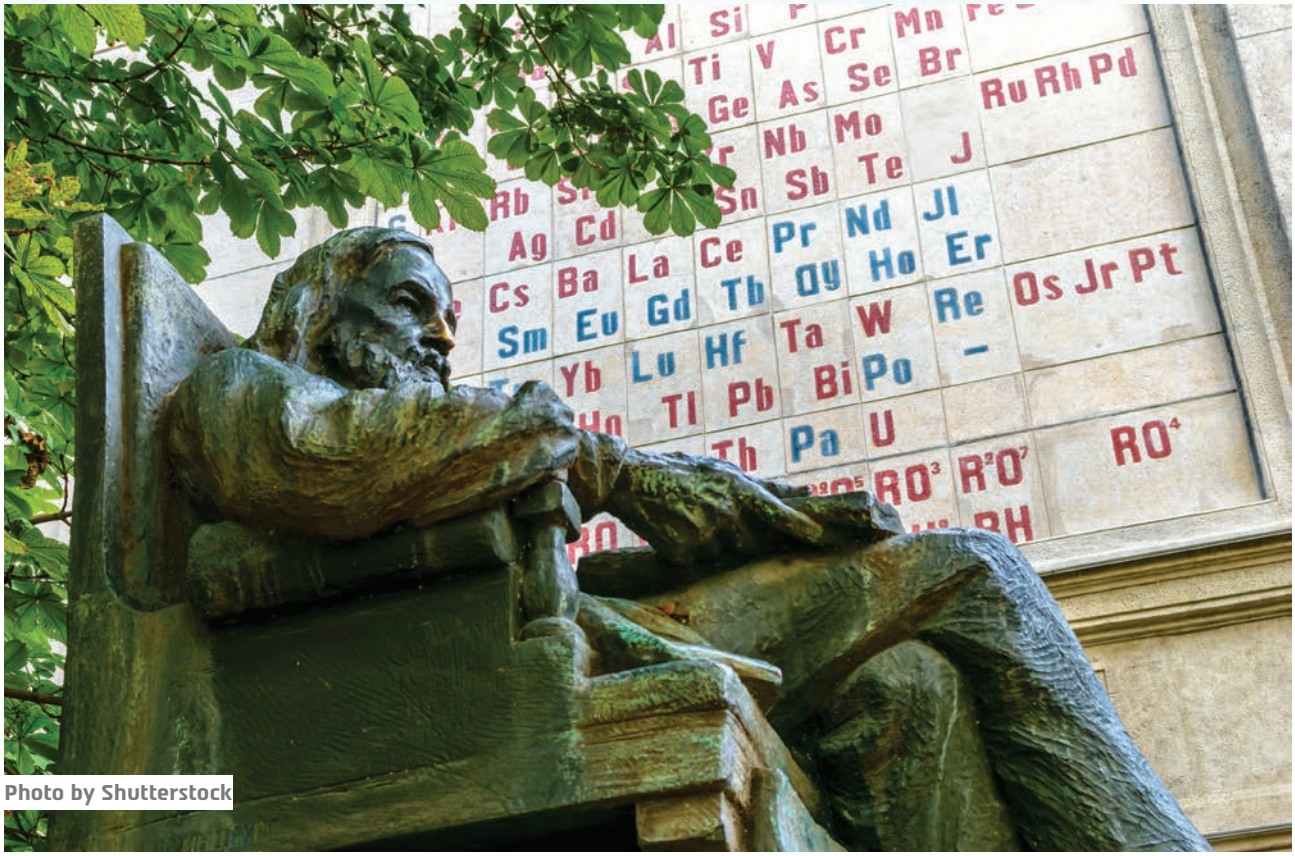

Photo by Shutterstock

Dmitri Mendeleev (1834-1907):
"Scientific sowing will rise for the harvest of the people"

thoroughly proved it. He displayed the law scientific meaning as the classification principle and a powerful instrument for further scientists. It is important that D. Mendeleev himself used the Periodic Law to correct atomic weights of certain elements and to predict three new elements: gallium, scandium and germanium. The greatness and philosophic meaning of the discovery of the Periodic Law and the Periodic Table is emphasized by the ongoing discoveries of new overweight elements, the latest of which is the element 118 that was called "oganeson" in honor of Russian academician Yury Oganesyan.

Another important scientific direction in the work of Dmitri Mendeleev was metrology. In the year 1892 Mendeleev has established the Main Chamber of Measures and Weights in Russia. Today its successor is the D.I. Mendeleev' Institute for Metrology in St. Petersburg, keeping the main metrological standards of Russia in the field of physico-chemical measurements.

Dmitry Mendeleev was a great scientist, a public figure, a teacher possessing the unique scope in the exploration of different sciences and areas of expertise. He was active in chemistry, physics, metrology, economics, technology, meteorology, chemical industry and even shipbuilding, published more than 350 papers, articles, brochures and books.

We would like to mention here only creation of white gunpowder, his cycle of lectures for students "The basis of chemistry", works on the development of petrochemical industry and glass blowing, works for study of solutions, and even the flight in a hot-air balloon in 1878.

Dmitri Mendeleev was recognized by scientists and scientific communities of many countries, awarded with memorable medals of the eminent scientists. The celebration of the International Year of the Periodic Table of Chemical Elements (IYPT 2019) allows to state that the work of D. Mendeleev is still remaining important, and to draw attention of the wide society to the diversity of chemical and metrological achievements and problems to be solved.

CITAC
Cooperation on International Traceability in Analytical Chemistry

VISIT A CITAC MEMBER AT HIS/HER LAB

METROLOGÍA DE MATERIALES AT CENAM, MEXICO

Y. Mitani, J.A. Salas-Tellez, M.Perez-Urquiza

Let's start the visit with the inauguration of the 10th metrology symposium for technological innovation and sustainable development organized by CENAM with the collaboration of several instrumental companies, laboratories associations and NMI partners.

The talks were focused on the specific needs in development of patterns and measurement methods, quality systems, standardization and conformity assessment, industrial applications, measurement traceability, technology transfer, validation of measurement procedures, education, efficient use of energy, redefinition of the international system of units, environment and biodiversity, agriculture and food, health, renewable energy, and climate change.

The 10th metrology symposium for technological innovation and sustainable development

This biannual symposium is one of the traditions established as a part of the missions of CENAM to outreach the importance of metrology and standardization. Several leaders in metrology and in analytical societies were invited, in particular the speakers in the chemistry area were Dr. Martin Milton, Director of the BIPM; Dr. Jin Seog Kim, Gas Analysis Working Group Leader; Dr. Zoltan Mester and Dr. Alan Steele from NRC; Dr. Walter Copan and Dr. John Lehman from NIST, Dr. Takashi Usuda from NMIJ. Other directors of NMIs with which close collaboration programs have been conducted took part in the symposium also. We had a strong program with over 111 technical speakers, with around 768 participants.

Activities successfully developed at CENAM in chemistry are: gas analysis program, inorganic analysis, organic analysis, electrochemical analysis and DNA analysis. Also surface analysis and recently nanometrology are under development, in accordance with the guidelines of CCQM.

After the 25 years of effort, CENAM maintains around 300 CMC and has developed nearly 500 CRMs, and maintains metrological services according to the CCQM guidelines, in which CENAM participates as member Institute, along with other 26 members, since 2004.

Currently the program is supported by 58 metrologist, and is dedicated to the method development, CRM development, standardization activities to support legal metrology, and regional trade safety issues, as well as to decreasing technical barriers to trade. For example, the CRM supporting quality of avocado for export, was developed in 2016 and recognized by the authority in 2017.

Substantial development of a laboratory network for the GMO detection and quantification (since 2001) was one of the models of collaboration with regulatory entities, having an inter-ministerial biosafety commission and a national laboratory network to determine GMOs. The network integrated 18 laboratories belonging to the ministries of agriculture, environment, health, economy, research centers, and universities, to support the safety program referring to the quantification of GMO at CENAM. Its capability in this field was achieved as a results of collaboration with NMIJ in 2009.

Preparing a candidate RM to determine pesticides in Avocado reference material

Another issue is development of reference measurement method using a new calibration system based on post-column reaction system. This development, being a result of the bilateral collaboration Mexico-Japan since 2011, supports the national environmental monitoring system of the environmental protection agency INECC. The capabilities related to the gas metrology, disseminated in the region of SIM since 2010, have been developed in collaboration with NIST and PTB since 1997. At the last symposium, as one of the parallel events the 39 meeting of the CCQM GAWG and M4SET project, supported by OAS, NIST and PTB and SIM, were conducted.

In the last 5 years CCQM has made a dramatic development, covering the needs of traceability in new fields of measurements in nano scale, DNA, protein and microbiological analysis. In this fields CENAM has been doing big efforts to develop reference methods and reference materials.

Dr. Yoshito Mitani, served many years as the Director General of Materials Metrology, has just retired from the Institute. The tasks of this position passed to the leadership of the new appointed manager - Dr. Melina Perez-Urquiza.

THE INORGANIC ANALYSIS LABORATORY OF THE NATIONAL METROLOGY INSTITUTE OF SOUTH AFRICA

Angelique Botha // NMISA, South Africa

The Inorganic Analysis Laboratory of the National Metrology Institute of South Africa (NMISA) has analytical capabilities in atomic spectrometric techniques such as inductively coupled plasma sectorfield mass spectrometry (ICP-SFMS) and inductively coupled plasma optical emission spectrometry (ICP-OES). The laboratory focuses on the development and maintenance of national measurement standards for the determination of major, minor, trace and ultra-trace elements in food matrices and environmental samples.

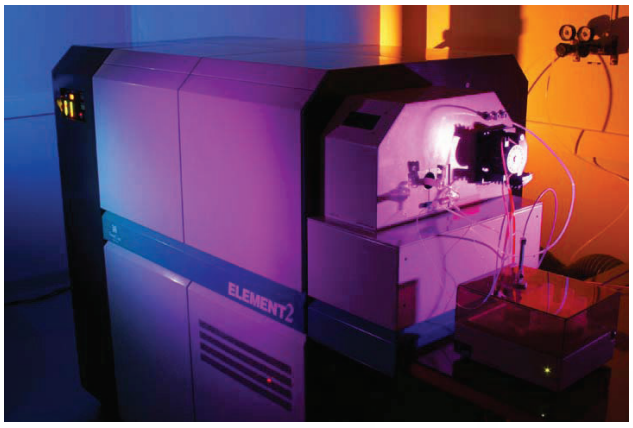

Figure 1: The inductively coupled plasma sectorfield mass spectrometer (ICP-SFMS) of the Inorganic Analysis Laboratory

Since 2000, the laboratory started participating in the international comparisons of the Consultative Committee for Metrology in Chemistry and Biology (CCQM) of the International Committee for Weights and Measures (CIPM). Over the years international measurement equivalence with other national metrology institutes (NMIs) and designated institutes (DIs) have been established in the field of the analysis of toxic and nutritional elements in food matrices, such as rice, wine and infant formula, as well as toxic elements in environmental samples, such as sediments and soils, plant material, plastics, etc.

The laboratory disseminates traceability to the SI units for metrology in chemistry to analytical laboratories in industry through the development of reference methods, reference measurements and the participation as reference laboratory in proficiency testing schemes. One such contract involves the value assignment of reference samples for nineteen (19) different inorganic elements in wheat flour samples produced in South Africa as well as imported samples. The project forms part of an annual crop survey performed by the Winter Cereal Trust of South Africa where the samples are used for trend analysis and as reference samples in quality control laboratories of different cooperatives across the country.

More recently, the laboratory, as part of a new initiative by NMISA, has also started to organise proficiency testing schemes in accordance with the requirements of the international standard ISO 17043. Currently, the

laboratory is assisting the Department of Health in South Africa through the organisation of a proficiency testing scheme for sodium in a range of food matrices from stock powder to bread, instant noodles, fat spread as well as cured meat products. The aim of the scheme is to improve the comparability between analytical laboratories in South Africa that analyse for sodium in food products in support of legislation that was promulgated recently for the reduction of the sodium content in a range of food products.

The laboratory has also participated as expert laboratory in a regional water testing proficiency testing scheme (the SADCMET Water Proficiency Testing Scheme) for many years. Here gravimetrically prepared water samples are analysed for 15 inorganic elements. The participation has grown to approximately 70 laboratories across Africa in 2018.

Plans are also underway to expand the capability of the laboratory into the realm of the production of matrix reference materials for toxic and nutritional elements in food matrices. The first candidate reference material for the characterisation of approximately twenty (20) toxic and nutritional elements in a wheat flour material has been prepared and packaged. The homogeneity and characterisation studies are currently underway. It is hoped that the material will be ready for the market by the end of 2019 and that the reference material certificate will contain certified values for most of the 20 elements. Plans are already in place to also develop certified reference materials (CRMs) for toxic and nutritional elements in white maize flour and cocoa powder.

The team of the Inorganic Analysis Laboratory is very small and consist of Dr Angelique Botha, who joined the laboratory in 2012 in the place of Mr Alex Barzev, our resident ICP-SFMS expert who retired and Ms Maré Linsky, who has already been a member of the team since 2001. Two students joined the laboratory in 2016 to allow the laboratory the opportunity to expand its capability into the field of organometallic speciation analysis. The first student, Ms. Magadima Thosago, joined the laboratory as an MSc-bursar in February 2016 and will soon finalise her project on the accurate

Figure 2: Maré Linsky and Angelique Botha preparing food samples for microwave assisted digestion

quantification of total arsenic and arsenic species in South African staple foods using ion chromatography (IC) coupled to inductively coupled plasma sectorfield mass spectrometry (ICP-SFMS).

The second student, Ms. Nwabisa Takata, first joined the laboratory as an intern and completed her MSc studies during her internship. In 2018, she started with her PhD-project, a life cycle study on the total selenium content as well as the selenium species found in two selected geographical regions of South Africa. The one region has selenium depleted soil resulting in vegetation with inherently low levels of selenium and live-stock that suffers from lethargy and low reproduction rates due to selenium deficiency. The second region has high levels of selenium in the soil, but low levels of selenium in the vegetation and livestock. It is hoped that the accurate quantification of the selenium species in the different soil and vegetation samples will shed light on the soil chemistry and the mechanisms involved with the uptake of selenium in the vegetation.

The Inorganic Analysis Laboratory also provides

Figure 3: Ms Nwabisa Takata, the PhD-student of the Inorganic Analysis Laboratory working on a project in selenium speciation in food and environmental samples

consultancy and analytical support to industry through method development for customers, training and analysis of ad-hoc samples. Ms Maré Linsky regularly presents an Uncertainty of Measurement Course for Analytical Chemists hosted by the National Laboratory Association of South Africa. She also serves on several working groups of the CCQM and is involved with some committee work of the South African Bureau of Standards (SABS) - assisting with standardisation issues for South Africa. Similarly, Dr Angelique Botha is actively involved in the work of the CCQM, currently being vice-chair of the KCWG, while also serving on several committees of the SABS and the International Organisation for Standardisation (ISO) where she is currently the chairperson of the ISO Committee for Reference Materials (ISO/REMCO). She is also a technical assessor for the ISO 17025, ISO 17043 and ISO 17034 international standards for the South African National Accreditation Service (SANAS) and several other international accreditation bodies.

CHEMICAL METROLOGY LABORATORY AT THE HEALTH SCIENCES AUTHORITY

Fransiska Dewi, Tang Lin Teo and Tong Kooi Lee //
Health Sciences Authority, Singapore

ESTABLISHING THE CHEMICAL METROLOGY INFRASTRUCTURE IN SINGAPORE

The Health Sciences Authority (HSA) is a Statutory Board under the Singapore's Ministry of Health. It is a multi-disciplinary agency which regulates health products, manages the national blood bank, and provides forensic medicine, forensic and analytical science services to support enforcement and regulatory agencies.

In 2008, the National Metrology Centre (NMC) of the Agency for Science, Technology and Research (A*STAR), the National Metrology Institute (NMI) of Singapore, partnered HSA to secure funding from the government to jointly establish the chemical metrology infrastructure in Singapore. NMC also designated HSA as a Designated Institute (DI) for chemical metrology in the areas of healthcare, medical science, food, pharmaceuticals & health products, and forensic, while it focuses on gas metrology. The infrastructure enables accurate and comparable chemical measurements to be made. These are important in international trade, and in areas such as food safety, environmental protection and healthcare, where decisions made are significantly influenced by the quality of measurements.

Following the designation, the Chemical Metrology Division (CMD) and its Chemical Metrology Laboratory (CML) were established within the Applied Sciences Group of HSA in August 2008 to develop the relevant measurement capabilities and spearhead the chemical metrology programme in HSA. To enable HSA to take on the chemical metrology role, the HSA Act was amended to include chemical metrology as one of its functions. This integrated well with the agency's multi-functional role.

DEVELOPING THE MEASUREMENT CAPABILITIES

At the initial phase, learning the skills quickly and developing the relevant measurement capabilities were the key challenges faced by CML. While we could draw on the analytical chemistry expertise already established within HSA, we had no experience on chemical metrology prior to the establishment of the laboratory. During these initial years, we received a lot of support from members of the chemical metrology community; many were members of CITAC before they retired. Through them, we were able to send our young scientists to established NMIs/DIs such as the National Measurement Institute, Australia (NMIA); National Institute of Metrology (NIM), China; National Institute of Standards and Technology (NIST), USA; Korea Research Institute of Standards and Science (KRISS), and LGC, UK for training and attachments. These training opportunities had helped us to acquire the relevant capabilities rapidly and provided the staff with the confidence to participate in regional and international comparisons.

We were indebted to Dr Robert Kaarls, Dr Willie May, Prof Yu Yadong, Dr So Hun Young and the late Dr Laurie Besley. It was Dr Kaarls who first invited us to the plenary meeting of the Consultative Committee for Amount of Substance – Metrology in Chemistry and Biology (CCQM) and the Working Group meetings as a guest of the President. He later led a team to conduct a peer review of our laboratory in 2011 and 2014, and made many suggestions to improve the quality and our work processes. Dr May had also helped us in many ways to develop and strengthen our measurement capabilities on clinical biomarkers. This has become one of our focus areas.

HSA participates actively in relevant CCQM and other Regional Metrology Organisation (RMO) comparisons to ensure that our measurement capabilities are equivalent to other established NMIs/DIs. Since 2009, the laboratory has participated in close to 50 CCQM/RMO Pilot Studies and Key Comparisons. These comparisons cover a wide area of work, which include adulterants, additives and contaminants in food, beverages and cosmetics, clinical biomarkers and elements in human sera, and purity assessment of organic compounds. HSA's results in the completed comparisons were comparable to those from established NMIs/DIs. These comparisons have provided us with the technical competence and confidence to launch new metrological services for our local testing laboratories. In recent years, HSA has also taken the initiative to organise/co-organise regional and international comparisons in the areas of food safety and healthcare. Four such comparisons have been organised/co-organised so far.

To date, HSA has 60 Calibration and Measurement Capabilities (CMCs) in the International Bureau of Weights and Measures (BIPM) Key Comparison Database (KCDB). These CMCs are in the areas of high purity chemicals, water, food, biological fluids and materials, and others (cosmetics).

LABORATORY FACILITIES

The laboratory is housed in a cleanroom with a rating of ISO Class 7 and has a wide array of instrumentation to support its measurement activities. A special "metal-free" section is created in the laboratory for inorganic analysis (see Figure 1). All furniture and laminar flow fumehoods in this section are custom-built and made of polypropylene which is resistant to acid.

Figure 1: "Metal-free" section in the laboratory dedicated for inorganic analysis

Major instruments used in the laboratory include NMR, high resolution ICP-MS, ICP-MS/MS, LC-ICP-MS, ICP-OES, LC-MS/MS, LC-QTOF, GC-MS/MS, LC-MS/DAD with fractional collector, HPLC-DAD, GC-FID/ECD and ASE (see Figure 2).

THE QUALITY SYSTEM

The quality system of CML is based on ISO/IEC 17025, ISO 17034 and ISO/IEC 17043. The laboratory was assessed thrice by a quality system expert from the Singapore

Accreditation Council (SAC) and peer reviewed by a team of experts from the international chemical metrology community in 2011, 2014 and 2018 (see Figure 3). CML is also accredited by SAC as a proficiency testing (PT) provider in accordance with ISO/IEC 17043 since August 2013. CML remains the first and only PT provider in Singapore.

Figure 2. High resolution ICP-MS

INTERNATIONAL & REGIONAL INVOLVEMENTS FOR INORGANIC MEASUREMENTS

HSA is actively involved in the chemical metrology community. At the international level, HSA is a member of the CCQM since 2014 and is actively involved in four of its working groups: Inorganic Analysis, Organic Analysis, Protein Analysis and Key Comparisons & CMC Quality. At the regional level, HSA is a full member of the Asia Pacific Metrology Programme (APMP) since 2008 and is involved in its Technical Committee for Amount of Substance (TCQM) and Technical Committee on Quality Systems (TCQS).

HSA is also an active member of the Joint Committee for Traceability in Laboratory Medicine (JCTLM). Two of our staff members serve as reviewers in the Database Working Group. Through our involvement in JCTLM, HSA contributes to international efforts on traceability in laboratory medicine. This, in turn, helps to strengthen and expand our metrological services to the clinical laboratories in Singapore.

In 2016, HSA together with its counterparts in the ASEAN region such as the National Institute of Metrology (Thailand) (NIMT) and Department of Chemistry, Malaysia (KIMIA) [with the support of the National Metrology Institute of Malaysia (NMIM)], initiated the formation of a new network, ASEAN Reference Material Network.

METROLOGICAL SERVICES OFFERED BY HSA

CML's current work focuses on inorganic, organic and protein/peptide analyses covering healthcare, food safety, pharmaceuticals and cosmetics, as well as purity assessment of organic compounds.

As a DI, HSA works closely with NMC to undertake the responsibility of disseminating metrological traceability to the local testing laboratories. Since 2011, HSA organises accuracy-based external quality assessment (EQA) and PT programmes for the local clinical and chemical testing laboratories, respectively. The assigned values for these programmes are independently determined by CML using high accuracy methods, and are traceable to the International System of Units (SI). Each assigned value is accompanied by its associated measurement uncertainty.

The HSA EQA programme was launched in 2011 to cover the healthcare area. It is an annual programme comprising two cycles per year to assist our local clinical laboratories uncover technical problems which their internal quality control processes may not pick up. The HSA programme focuses on biomarkers of chronic diseases affecting the Singapore population such as diabetes mellitus, heart and kidney diseases. It currently covers 17 clinical markers. The HSA programme provides an objective evaluation of the accuracy of clinical measurements for these biomarkers, and also serves as a platform to assess the comparability of the test results of the local clinical laboratories. The HSA EQA programme is well participated by all the public clinical laboratories and almost all the private clinical laboratories in Singapore. In 2019, a dedicated EQA programme using fresh human whole blood for haemoglobin $A1_c$ (HbA1c), a biomarker for diabetes mellitus, will be launched.

HSA currently organises two PT schemes a year comprising multiple inorganic or organic contaminants or additives in various food and aqueous-based matrices to assist our local chemical testing laboratories in ensuring the quality of their results. The PT schemes are designed to address relevant issues related to food safety, water quality and cosmetics. They are organised with the aim of providing metrological traceability to participating local laboratories, enabling them to assess

Figure 3. CML's staff members with peer reviewers, Dr Akiko Takatsu, National Metrology Institute of Japan (NMIJ) and Dr Byungjoo Kim, KRISS (left), and Inorganic Chemistry Team with Dr Mike Sargent, LGC (right) in March 2018

the accuracy and comparability of their test results.

At the end of each EQA or PT programme, HSA organises symposium or forum/ discussion session to provide feedback and recommendations to participating laboratories on ways to improve measurements and the estimation of measurement uncertainties. To further raise the understanding of the importance of chemical metrology, HSA, together with NMC and SAC, regularly organise seminars and lectures to share their experience and knowledge with the industry, academics and stakeholders. Since 2014, CML has conducted training courses on basic statistical tools, method validation and measurement uncertainty for the local testing laboratories. About 600 laboratory personnel have so far been trained.

In addition, CML provided trainings to its counterparts under the Metrology - Enabling Developing Economies in Asia (MEDEA) programme in the organic and inorganic chemistry areas. MEDEA is a programme initiated under the APMP-Physikalisch-Technische Bundesanstalt (PTB) MoU with the aim of strengthening the development of metrology in the developing economies of the region.

CML produces a list of CRMs which can be used by the testing laboratories as calibrants and quality controls, as well as for method validation. CML maintains clinical CRMs in the biological matrices such as human serum, haemolysate and urine, covering about 20 clinical biomarkers with different concentration levels. CML also maintains CRMs in the form of pure substance and matrix materials (e.g. soy sauce, mushroom powder, juice, water, cosmetic cream and lipstick). These CRMs are monitored regularly to ensure the long term stability of their reference values.

MOVING FORWARD

CML is continuously developing its measurement capabilities in new areas of importance. In the area of healthcare, CML is building its measurement capabilities in the more challenging clinical biomarkers. These include steroid hormones in human serum and low density lipoprotein (LDL) subclass testing; the use of signature peptides as calibrants; and complex proteins in human serum such as human growth hormone, haemoglobin variants and procalcitonin. Some of these efforts are in line with Singapore's fight against diabetes through strengthening the reliability of HbA1c measurement for diabetic patients, as well as with the international standardisation efforts for priority clinical biomarkers through participation in the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC) Working Group. To keep pace with healthcare transformation, CML is expanding the HSA EQA Programme to cover point-of-care devices using fresh human whole blood samples as EQA materials.

In the area of food safety, pharmaceuticals and cosmetics, CML is also building its capabilities in the measurement of mycotoxins and veterinary drug residues in food, as well as nanoparticles in food and cosmetics. In 2018, CML sent one of its staff members for training and attachment at NIM, China to strengthen its capabilities in the area of mycotoxin measurements. HSA will continue to develop its capabilities to address consumers' safety concerns.

CITAC
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MESSAGES OF THE NEW MEMBERS

PAOLA FISICARO

LNE, France

I started my career in metrology in chemistry in 2003 at INRIM, developing primary standards for pH measurements. I did not abandon this activity when I moved to LNE in 2007, where I have been working to promote pH standards not only in "classical" media such as buffer solutions, but also in "complex" media such as organic solvents and seawater.

At LNE I have also been engaged in developing inorganic analyses, such as elemental and speciation analyses and I am currently vice-chair of the Inorganic Analyses Working Group of the CCQM.

I have always been keen to apply and promote the principles of metrology, in order to disseminate them among different communities. This is the reason why, with my team of passionate researchers in chemistry, I am active in collaborate with a wide range of stakeholders. In particular, I have well-established collaboration with stakeholders in the oceanographic community, being co-chair of the European Metrology Network for Climate and Ocean observation, currently chairing the ocean observation section. I am also active in promoting the MIC concepts in the emerging area of nanoparticle characterisation applied in different fields such as environment, food and biological samples. For this reason I have started to collaborate with several scientists in the field of toxicology and nanomedicine to support their studies with reliable data.

CITAC is one of the key players in the area of MIC, promoting metrological traceability leading to more reliable decisions.

I have been honoured to be selected as a member of CITAC and I look forward to fruitful interactions with CITAC members and to providing an active contribution in CITAC activities.

TONY DADAMOS

Educational Foundation of Fernandópolis, Brazil

I am very proud from been elected and be part of CITAC from 2018. I have always seen CITAC as a reference institution in the world and composed of respected professionals in the area of metrology. And today I feel lucky to be a member of this institute.

I met metrology in my master's degree, applying concepts of uncertainty in clinical and food measurements. It was the first moment that I fell in love with metrology. Although it was just a passion I wanted to know if it could become love. For this during the PhD course I invested in deepening my knowledge in metrology by taking my course at University of State of São Paulo (Brazil) and University of Lisbon (Portugal), as well as specialization courses in Brazil and Europe. I would like to thank Prof Dr Ricardo Silva who was and still are my greatest incentive in expanding my knowledge in metrology.

Measurements, traceability and trade can not be carried out without metrological knowledge, that is why metrology is an exciting area. I am currently investing in the research and development of new approaches to calibration curves and their calculation of uncertainty using bottom-up approach and Monte-Carlo simulations methods at the University of State of São Paulo and Educational Foundation of Fernandópolis that I am currently teaching. I am a partner of SPR Consulting and Quality Training, in which we work in physical metrology with physical calibration laboratories working in the clinical and hospital areas, and in chemical metrology we are developing reference material for environmental and forensic area.

In all my researches I would like to emphasize a little bit about chemical metrology and the importance of reference materials, which one in Brazil, in particular, is a big problem. Brazil has continental dimensions with more than 1000 laboratories accredited by the local NMI (Inmetro), but only nine laboratories accredited to produce these materials, having a deficit of production and having the necessity to import these products. The development and production of certified reference materials is a major challenge. The new norms and policies increasingly directed to the quality management system have required these materials and the responsible NMI has supervised the proper use from all of them, increasing the demand and consequently the commercialization. Certified Reference Material is required in the validation of procedures, uncertainty estimation, routine controls of laboratories in various areas of practice, and proficiency testing of laboratories that have implemented or intend to implement quality management systems and must ensure traceability according to the guidelines of ISO/IEC 17025: 2017. Due to this problem that affects several countries of the world, I intend to invest all metrological knowledge to develop these products.

And with the support of CITAC and all its members, we can disseminate and extend the concepts and importance of metrology to all countries in the world. With this I intend to launch larger flights in metrology and I hope to actively contribute to the actions of CITAC over the years.

JORGE EDUARDO DE SOUZA SARKIS

Institute of Energy and Nuclear Research, Brazil

I started my studies in Metrology in the beginning the decade of 1980, as a PhD student in nuclear chemistry, in the Institute of Transuranium Elements, Karlsruhe, Germany, when I had the honor and privilege to meet, for the first time personally, Professor Paul de Bievre. Paul was an enthusiastic leader in chemical metrology... Once he said "Definitions of metrological concepts are lighthouses which are clarifying our communication about results of chemical measurements". In my modest opinion, he was one of the most important "lighthouses" in metrology spreading his light anywhere he was able. At that time, we were focused in the establishment of target values for the main analytical assays used in the nuclear industry. The discussions were around the state of art and state of practice of each technique for each specific application. There was a huge and detailed work, which gave me a broad vision of a large number of techniques and the opportunity to meet several specialists around the world establishing a fruitful network in analytical chemistry.

Returning to Brazil, I started to organize the Laboratory of Chemical and Isotopic Analysis, following at this time modern recommendations of laboratory best practices and establishing QA/QC programs. The era of trace and ultratrace analysis was just at its beginning, requiring specific infrastructure, suitable measuring devices and instruments. Ultratrace analysis cannot be conceived without a metrological development.

In 1990, I was appointed as the Brazilian Coordinator of the program "Production and Certification of Certified Reference Material - Uranium Oxide" for the Brazilian-Argentine Agency for Accounting and Control of Nuclear Materials, under nuclear cooperation program for the Peaceful Use of Nuclear Energy, signed by Argentina and Brazil. Thus, with the extraordinary collaboration between professionals, using the available infrastructure in both the countries, four materials were produced with different enrichments for beginning. Ten years later I returned in this theme in collaboration with Paul de Bievre, supervising a PhD thesis, in which a set of ten uranium hexafluoride isotope reference materials in the range from 0.5 to 20% mass of 235U were prepared, characterized and certified. At the same period, I started my academic activities as Associated Professor at São Paulo's University (IPEN - Nuclear Technology Program) and had the opportunity to disseminate, mainly to the new generations of analytical chemists, important concepts of metrology.

In 2005, our laboratory was accredited by the National Institute of Metrology, Standardization and Industrial Quality to ISO/IEC 17025 standard. It was the eighth Laboratory in Brazil accredited to this standard. I have also been the Coordinator of a national intercomparison analytical program, involving 7 national laboratories, in cooperation with Ministry of Agriculture, Livestock and Food Supply, for metals in fish tissues. During the last years I've been involved in forensic and environmental metrology. Both the areas are paramount aspects of welfare for the society and demand development of several metrological standards. More recently, I was invited to join the Eurachem/CITAC Working Group for development of the second edition of the guide "Measurement uncertainty arising from sampling. A guide to methods and approaches".

It has been a long journey. Therefore, I feel myself honored to have now the opportunity to join CITAC, participate in its activities and contribute to the development and dissemination of metrology.

NARINE OGANYAN

VNIIFTRI, Russia

First of all, I would like to thank CITAC members, who have accepted me into their family, and of course Samuel Wunderli, nominated me for that.

I have received the M.Sc. degree from the Polytechnic Institute of Yerevan (the Faculty of "Chemical Technology," 1985), and Ph.D. from D. Mendeleev Institute of Chemical Technology (1992), Moscow, Russia. In 1985 – 1994 I was a researcher at the Chemical Agents Factory, Institute of Applied Chemistry, Chemincor Co., Armenia. I have worked in the field of synthesis of organic reagents and realized how difficult it is to analyze the synthesis products. In that time, nobody in my surrounding knows about metrology in chemistry.

I have started to work as a metrologist since 2006, liked this job from beginning and like it now also. In 2006 - 2014 I was Head of Service of Research and Metrology Support at the NMI, Armenia, Quality Manager of the NMI and National Secretary of COOMET, then since 2016 - Deputy Head of Physical-Chemical and Electrical Measurements Departments of All-Russian Research Institute of Physico-technical and Radio-technical Measurements (VNIIFTRI), Russia. I am actively involved in the development of various documents and recommendations in the field of metrology in chemistry and biology.

I was a member of TC 1.12 "Reference Maerials", TC 3.1 "Quality Forum", TC 4 "Information and Training" of COOMET, an expert in TC 2 "Legal metrology" of COOMET (for 7 years), the co-coordinator of COOMET project 543/AM/11 "Development and administration the database of reference materials of COOMET", the expert of National accreditation body of Armenia, the Chairman of the Subcommittee "Metrology, standardization, certification, products quality" of the Financial Economic and Budget Committee of the Public Council of Armenia, the Chairman of the State Examination Commission at the Armenian National Agrarian University, Chair of Food Technology, Specialization "Testing, certification and standardization."

Our VNIIFTRI team is active at CCQM Working Groups (KCWG, IAWG, EAWG, GAWG). We are revising the international recommendation OIML R54 "pH scale for aqueous solutions" and are developing a new OIML Recommendation for the pH measurement area. I am also a reviewer of the Russian Journal "Reference Materials" and the Chairman of the electrochemical measurements commission at Rosstandart, Russia. Our team organizes conferences on Metrology in the field of physicochemical measurements, and the next Conference will be held 17-19 Sep 2019 in Suzdal, Russia. I invite CITAC members to take part in this Conference.

I hope that my activity at CITAC will contribute to measurement traceability in Chemistry and Biology, as well as in the fields of their technical applications.

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MEETING REPORTS

3RD INTERNATIONAL SCIENTIFIC CONFERENCE "REFERNCE MATERIALS IN MEASUREMENT AND TECHNOLOGY"

Ekaterinburg, Russia, 11-14 September

O.N. Kremleva and N.S. Taraeva // Ural Research Institute for Metrology (UNIIM), Ekaterinburg, Russia

The IIIrd International Scientific Conference "Reference Materials in Measurement and Technology" was held in September 2018 in Ekaterinburg. This event was organized by

Federal Agency on Technical Regulating and Metrology (Rosstandart) and the Scientific Methodological Center of Reference Material State Service, **Ural Research Institute for Metrology (UNIIM).** The priority task of the Conference was the creation of an open forum for exchanging scientific information on fundamental and applied research in the field of reference materials, as well as the promotion of reference materials as a technical, regulatory and methodological basis, needed to ensure the measurement quality.

Dr. Sergey Medvedevskikh, the UNIIM Director and Chairman of the Conference Organizing Committee, pointed out that the Conference gave an answer to the issue related to the digital transformation of the economy, social sphere and, in general, quality infrastructure in our country, as well as in partner countries. Ensuring the uniformity of measurements is one of the main tools in development of innovative areas. At the same time the operation of the system for ensuring the uniformity of measurements itself is also experiencing a rapid transformation to "digit".

"One of the problems of this transformation is the continuous improvement of the processes associated with the collection, processing, storage and dissemination of data", said Sergey Medvedevskikh. "An increasing number of users in Russia and abroad need availability of reference materials (RMs), including development of new RMs with regards to global digitalization. This means for us continuous optimization of mechanisms of investigation and forecasting the needs in metrological support, including the use of reference materials. Along the way, there are the challenges of RM globalization on the international market and, of course, of increasing their competitiveness".

Leading experts from different countries are working towards the solution of these issues. The Conference in Ekaterinburg was attended by scientists, teachers and postgraduate students from universities, experts from research metrology institutes, enterprises and organizations of the industrial sector, representatives of international and interregional organizations, such as ISO/REMCO, CITAC, COOMET, the Central Secretariat of international RM data base COMAR, experts in the area of RMs from Belarus, Germany, Israel, Kazakhstan, Netherlands, Poland, Russia, South Africa, Switzerland and USA.

The Conference hosted 11 special scientific sections. 80 scientific contributions were represented at the conference plenary, special and poster sections. Contributions of the representatives of state scientific metrology institutes within the Rosstandart system and reference material producers took a significant part of the Conference program. They were interesting for the participants, dealing with the issues of the formation and implementation of state policy of the countries in the field of ensuring the uniformity of measurements. The results of research in the development and production of reference materials, as well as their practical application in various fields were attractive for the audience also. The growing interest to the development of reference materials in the field of health and pharmacology was noted. The issues of development of reference materials for maintaining automated measurement processes were considered. Within the framework of the Conference the issues of interlaboratory comparisons, including those with the use of reference materials were addressed as a separate flow.

The International Section started from the contribution by Angelique Botha, Chair of ISO/REMCO, National Metrology Institute of South Africa (NMISA), addressed the issues of ISO/REMCO activity concerning the development and revision of international documents on reference materials. The contributions of foreign colleagues, highlighting trends in the development, production and use of reference materials were also heard with a great interest.

Publication of the Conference proceedings "Reference materials in measurement and technology" is planned by Springer. The contribution of the Conference participants and more detailed information on the event are available on the Conference website www.conference.gsso.ru.

IUPAC/CITAC WORKSHOP "QUALITY OF CHEMICAL ANALYTICAL TEST RESULTS FOR CONFORMITY ASSESSMENT OF A MATERIAL OR OBJECT"

Tel Aviv, Israel, 21 Jan 2019

Ilya Kuselman // Independent Consultant on Metrology, Israel

The workshop has been organized by IUPAC and CITAC as a milestone of the IUPAC project 2018-004-1-500 "IUPAC/CITAC Guide for evaluation of risks of conformity assessment of a multicomponent material or object due to measurement uncertainty". The Israel Analytical Chemistry Society and Israel Laboratory Accreditation Authority (ISRAC) took part in the event preparation, Merck and Bioforum companies supported it.

After welcoming by Dr. Ilya Kuselman, Independent Consultant on Metrology, Israel, Chairman of the Workshop International Advisory Committee; Prof. Érico Flores, University of Santa Maria, Brazil, Vice-President of the IUPAC Analytical Chemistry Division; and Dr. Michela Sega, National Institute for Research in Metrology (INRIM), Italy, Chair of CITAC, the workshop started from the plenary lecture by Em. Prof. D. Brynn Hibbert, UNSW Sydney, Australia. This lecture was dedicated to evaluating and using big data in chemistry. 'Big data' might be the multi-dimensional output of GC-MS-MS that needs to be calibrated to solve a multivariate problem. To the pharmaceutical or organic chemist integrating NMR with finding targets in a database that might have biological activity the use of 'big data' is now almost routine. For the relatively new branch of cheminformatics it might be trawling through clicks on published articles across the world to decide what the trending areas of chemistry are this week. In fact data becomes 'big' as soon as one person cannot understand them all at one view. If a chemist must resort to a computer to treat the flow of information from an instrument, then the data is already 'big' whether a few kilobytes, megabytes or terabytes. IUPAC is "the world authority on ... atomic weights and many other critically-evaluated data" (https://iupac.org/what-we-do/). When the data to be evaluated are pouring in from the vast amount of peer-reviewed (and quasi-peer reviewed) literature, we need new tools to reduce, visualise and extract useful information from it.

The next lecture was by Mr. Steve Sidney, National Laboratory Association, South Africa, on the International Laboratory Accreditation Cooperation (ILAC) mechanism to provide quality test results. This presentation was focused on how the cooperation works, how differing approaches are evaluated and how ultimately the economies represented by the cooperation have benefited.

In the lecture by Dr. Ilya Kuselman on conformity assessment standards, he talked on the Committee on Conformity Assessment, ISO/CASCO, and its standards,

Figure 1: IUPAC project team on the way to the Dead Sea

most relevant for a chemical analytical laboratory: ISO/IEC 17000:2004 (vocabulary and general principles),

ISO/IEC 17025:2017 (requirements for testing and calibration laboratories), ISO 17034:2016 (requirements for reference material producers), and ISO/IEC 17043:2010 (requirements for proficiency testing). In this lecture ILAC G8 guidelines draft was also discussed and some other international documents on decision making in conformity assessment taking into account measurement uncertainty (JCGM 106, Eurachem/CITAC, EURAMET, IUPAC), important in the field.

Dr. Francesca Pennecchi, INRIM, Italy, gave a lecture on risks of false decisions in conformity assessment. In order to calculate such risks, the basic idea underlying in the ISO/IEC Guide 98-4:2012 (JCGM 106) is to resort to probability theory: the knowledge about the measurand can be expressed in terms of a probability density function, which according to the Bayes theorem, combines prior information on the measurand and new knowledge (including the uncertainty term) acquired during the measurement. In this vein, the IUPAC/CITAC guide for investigating out-of-specification test results of chemical composition was published in 2012. The IUPAC projects devoted to the evaluation of probability of false decisions in conformity assessment of multicomponent materials or objects were performed recently and corresponding IUPAC/CITAC Guide draft will be circulated for comments soon.

Prof. Ricardo Bettencourt da Silva, University of Lisbon, Portugal, reported on setting data requirements. In the lecture he concentrated on the data required to ensure that a measurement result is fit for purpose, and a measurement procedure is producing fit for purpose results. The fitness for purpose is achieved when the measurement uncertainty is small enough to allow conclusive decisions on the tested items. A target (maximum admissible) measurement uncertainty should be defined to allow an objective and transparent decision about the adequacy of the measurements.

A short presentation "Proficiency testing and interlaboratory comparisons as a tool for accreditation" was given by Dr. Ori Elad, ISRAC, Israel, in the time of the first round-table discussion, moderated by Dr. Michela Sega. Laboratories accredited under the ISO/IEC 17025 and ISO 15189 standards are under obligation to routinely monitor and ensure the validity of the results reported. One of the means for that is proficiency testing (PT) and interlaboratory comparisons (ILC). In this presentation Dr. Elad has explained the purpose of PT and ILC, the differences between them, their role in quality management and the factors that should be taken into account when deciding on the frequency and level of participation in them according to the policy of ILAC and ISRAC.

Figure 2: Visiting the Israeli police headquarters in Jerusalem

Another short presentation "Measurement uncertainty and risks of false decisions in conformity assessment" was delivered at the same round-table discussion by Dr. Narine Oganyan, All-Russian Research Institute of Physico-technical and Radio-technical Measurements (VNIIFTRI), Russia. She said that in the majority of cases conformity assessment is based on measurement results, since measurement results are considered as the main source of information about the characteristics of any object. When measurement uncertainty is large, the probability of a false decision in conformity assessment is large also.

The first lecture after the lunch was "Databases for proficiency testing schemes and certified reference materials - EPTIS and COMAR" by Dr. Johannes van de Kreeke, Federal Institute for Materials Research and Testing (BAM), Germany. He said that the PT scene is changing rapidly. PT providers merge, hybrids of PT and RM appear and closed ecosystems squeeze independent providers out of the market. The RM market is very much comparable to the PT market, but larger. Its

growth is impressive, extensive company and reseller portfolios suggest that availability of RMs is no longer an issue. Many materials seem to have become true commodities indeed, and this segment of the market is very profitable. EPTIS (a database for PT schemes) and the new COMAR (a database for CRMs) aim to bring valuable and challenging non-routine resources to the fore.

Prof. Érico Flores gave a lecture on risks and new possibilities in sample preparation for further halogens determination in organic matrices. He highlighted that the digestion efficiency of some systems for sample preparation is limited for many matrices, especially for further halogens determination. Even using microwave-assisted closed vessels, some drawbacks can occur and incompleteness of digestion/extraction has been frequently reported. There is a necessity for development of methods with lower reagent consumption, less analytical steps and lower waste generation combined with high efficiency of digestion.

Dr. Simcha Simron, Division of Identification and Forensic Science (DIFS), Israeli Police, presented a lecture on detection and identification of drugs – the challenges of meeting scientific and legislative standards. Scientific evidence plays a key role in modern day courtrooms. Exhibits from crime scenes are collected and analyzed by the experts of DIFS. Reports given by DIFS experts are usually a product of a laborious and meticulous process. The analysis must meet scientific standards as well as judicial requirements. In recent years there has been a growing demand for higher QA standards in all aspects of forensic operations. In fact, the DIFS has undergone accreditation by ISRAC. As part of the DIFS, the National Drug Laboratory deals with analyzing and identifying exhibits that are suspected of containing illicit drugs. The identification is based on at least two independent matching scientific results. In accordance with the Israeli dangerous drugs ordinance, the results of exhibit examinations are qualitative analyses results.

Dr. Markus Obkircher, Reference Materials R&D, Merck, Switzerland, explained the Merck strategy in development of RMs for specific tasks and applications. Merck installed centers of excellence as R&D teams developing customer specific solutions as well as new catalog products, providing global access to RMs for many different market segments. In his lecture Dr. Obkircher gave short background for understanding the most relevant metrology aspects during a RM preparation and characterization, presented an overview of the different reference methods used in the certification processes.

Dr. Orna Dreazen, Nextar Chempharma Solutions Ltd, Israel, reported on challenges in determination of active pharmaceutical ingredients and their stability in cannabis based drug products. Use of cannabis is documented for over 6000 years in different cultures. People using it are exposed to highly variable content of cannabinoids and other types of molecules. Therefore, health authorities encourage the pharmaceutical companies to develop standardized pharmaceuticals for the benefit of patients and to support evidence based decisions. Plant derived products may either contain whole plant extracts (botanical drugs) or individual plant derived molecules. The problems of testing botanical drugs for the active ingredients, and of establishment of the drugs stability indicating methods were discussed in this lecture.

The second round–table discussion moderated by Dr. Raphy Bar, BR Consulting, Israel, was started from a short presentation by Prof. Mikhail Okrepilov, D.I. Mendeleev Institute for Metrology (VNIIM), Russia, on metrology of the alcohol control in breath of a vechicle driver. Prof. Okrepilov said that the legislative limit of the alcohol concentration in a driver breath in Russia is 0.16 mg/L. More than 15 different types of breath alcohol analyzers of Russian and foreign producers are in use in the Russian Federation. A generator of vapor-gas mixtures in combination with CRMs of aqueous solutions of ethanol, as well as CRMs of composition of gas mixtures in cylinders under pressure are used for certification and calibration (verification) of breath alcohol analyzers. Metrological centers use both CRMs of aqueous solutions of ethanol and gas mixtures in cylinders under pressure, produced in Russia. VNIIM has developed and maintaining corresponding state primary measurement standard for units of molar fraction and mass concentration of components in gaseous medium, and participates in the international key comparisons in this field.

Next day, 22 Jan 2019, paricipants of the workshop took part in the Metrology, Quality and Chemometrics sessions of the Isranalytica Conference and Exhibition. A total of more than 3600 chemists visited the exhibition, about 1000 of them were registered at the conference. However, about 30 only colleagues were interested in the workshop and in the Metrology, Quality and Chemometrics sessions. Probably the number of quality managers and metrologists of laboratories is so minor in comparison with the number of all the laboratory staff, or they were not attracted by our events and their topics. Anyway, it is a phenomenon which should be more analyzed further and understood.

After the work, a trip to Dead Sea was organized: on the picture the IUPAC project team is near Jericho (from the left: I.Kuselman, F. Pennecchi, R. da Silva and D.B. Brynn).

Also visits to DIFS, Israeli Police, and the Water Institute at Tel Aviv University were very interesting. On the next picture there are some workshop lecturers at the Israeli Police Headquarters in Jerusalem.

15TH INTERNATIONAL SYMPOSIUM ON BIOLOGICAL AND ENVIRONMENTAL REFERENCE MATERIALS (BERM15)

Markus Obkircher // Sigma-Aldrich Production GmbH, Switzerland

The 15th International Symposium on Biological and Environmental Reference Materials (BERM15) was held at the Erwin Schrödinger Centre of Humboldt-University in Berlin, Germany on September 23-26, 2018.

In the early 1980s several changes and improvements of analytical capabilities took analytical chemistry, biochemistry and metrology into a regulated and accredited environment. Several scientists and researcher recognized that a new global business for testing laboratories accreditation and for reference materials producers was created. The need to have discussions around the production of matrix reference materials to support chemical analyses of biological materials let to the first BRM (Biological Reference Materials) that took place in Philadelphia in September 1983 with 25 participants sharing research results on food and nutrition analysis. Since its origins BRM has not only evolved to BERM but also extended its reach over a 36-year lifespan now touching almost every aspect of chemical measurement. While Certified Reference Materials (CRMs) and their preparation, use and availability have always been at the heart of the Symposium, related topics such as Quality Control Materials (QCM), Proficiency Testing (PT) and Accreditation were covered as well.

While BERM14 in 2015 in Maryland was attended by a record number of nearly 300 participants from 28 countries, BERM15 was much smaller with 130 attendees. Instead of a 4-day symposium with parallel oral sessions the organizers chose to have only one presentation stream for three days.

Host and local organizer was the Bundesanstalt für Materialforschung und prüfung (BAM). The local organizing committee was led by Sebastian Recknagel and Matthias Koch from BAM, the members of the scientific committee represented 8 different institutions from 7 countries: Ulrich Panne (BAM, Germany), Kathrin Breitruck (SIAL, Switzerland), Angelique Botha (NMISA, South Africa), Stephen Ellison (LGC, UK), Doris Florian (JRC, Belgium), Bernd Güttler (PTB, Germany), Markus Obkircher (SIAL, Switzerland), Catherine Rimmer (NIST, USA), Takeshi Saito (NMIJ, Japan), Mike Sargent (LGC,

UK), Stefanie Trapmann (JRC, Belgium), Steven Wise (NIST, USA). This committee supported the creation of the scientific program that included different focus areas with a total of 12 keynote presentations in 11 morning and afternoon sessions.

After a warm welcome by Ulrich Panne (BAM), the symposium opened with a keynote lecture by Yannic Ramaye (JRC) on the production and certification of materials for electrophoretic mobility/zeta potential measurements. He eluded interlaboratory experiments that were conducted to derive the zeta potential for two different primary reference materials. The second keynote speaker of the session on "CRMs for Industry and Nanomaterials and challenges in Reference Material Preparation" was Jeremy Melanson (NRC) who displayed recent results as well as legal and regulatory hurdles in the development of Cannabis certified reference materials. Further presentations this session were Rainer Schramm (Fluxana) on the production of new industrial CRMs for X-ray fluorescence analysis and Jens Boertz (LGC) who gave a general overview on potential challanges during the preparation of certified reference materials. Steffen Uhlig (QuoData) presented latest results on outlier identification in proficiency testing experiments and the use of robust statistics such as measurement uncertainty-weighted Hampel means. Mark Lewin (NMIA) addressed the assignment of reference values for endocrine hormones in human serum using 2D LC-MS/MS and Debra Ellisor (NIST) eluded the process for generating custom cryogenic reference materials by application of small-batch amendment.

In the keynote presentation of the session "RM Standards – a new landscape", Angelique Botha (NMISA) went into details of new ISO Guides 85, 86, 80, and most importantly the ISO Guide 33 that was published in 2015. She explained the different changes in the new editions and promoted several the guidance documents that were developed by ISO/REMCO. The session continued with presentations by Stephen Ellison (LGC) on the assessment of homogeneity and stability provisions in ISO standards and Adriaan van der Veen (VSL) on Bayesian methods in the certification of gaseous reference materials. After Gill Holcombe (LGC) presented the transformation ISO Guide 34 to ISO 17034 accreditation and the consequences for reference materials producer, the session concluded with the contribution of Johannes van de Kreeke who showcased the COMAR database platform that was established at BAM and contains more than 100'000 reference materials entries.

The session "Certification of pure RMs – Traceability and uncertainty" was led off by Takeshi Saito (NMIJ). He showed the current challenges in an accurate characterization of small organic molecules and described minimum requirements for homogeneity, stability and establishment of the traceability. John Warren (LGC) presented his research of purity determination of peptides by quantitative NMR and Markus Obkircher (Merck) explained the results of a round robin experiment, in which ^{1}H, ^{19}F, ^{31}P qNMR was used to establish a mean value for different analytes. Iris de Krom (VSL) eluded on the approaches for purity assessment of high-purity gases

Best poster award for Benilda Ebarvia from the National Metrology Laboratory Philippines

through a standard addition method and application of Bayesian calculation models. A panel discussion on the implementation of new guidelines concluded the first day.

The first sessions of the second day on "CRM Developments for Food and Dietary Supplements" and "Reference Materials for Health, Pharmaceuticals and Bioanalysis" included key note lectures from Darryl Sullivan (Covance Laboratories) on the process, development and use of SRMs for infant formula testing and Pearse McCarron (NRC) on the algal toxin CRMs. Darryl Sullivan outlined the panel process of the AOAC stakeholders (SPIFAN) and the new AOAC standard development process for standard method performance requirements, Pearse McCarron presented the history at NRC in developing multiple standards in the field of marine biotoxins, a topic that was further eluded in detail by Daniel Beach (NRC) who addressed untargeted HR-MS approaches for profiling and stability assessment of those compounds. Further presentations in these sessions were given by Berit Sejerøe-Olsen (JRC) on pesticides in food matrices, Joonhee Lee (KRISS) on the development of CRMs for nutrients in food, Catherine Rimmer (NIST) on reference materials for dietary supplement measurement support, Karen Phinney (NIST) on new tools for the characterization of proteins as CRMs, Paula Brown (British Columbia Institute of Technology) on the role of CRM in Metabolomics natural product research and Joseph Betz (NIH) on the use of CRMs in basic biomedical research. The session was completed by Sarah Hill (LGC), Matthias Weber (EDQM) and Enea Pagliano (NRC) who presented the quantification of iodine in complex matrices, the adoption of the new guideline ICH Q3D on elemental impurities for the control and the development of a new CRM for nitrate in spinach powder by using isotope dilution MS.

The other long session of the second day focused on "CRM Developments in Environmental Analysis" ,"Isotopes in Natural Matrix Reference Materials" and "Speciation Analysis and Reference Materials". Key note speakers were Robert Vocke (NIST) who presented isotope ratio measurement scales with regards to the new SI unit definition and Kazumi Inagaki (NMIJ) who displayed the process at NMIJ to ensure the reliability of speciation CRMs using different extraction and measurement techniques such as LC-ICP-MS, GC/MS and GC-ICP-MS.

Further presentations in this combined session included contributions from Dmitriy Malinovskiy (LGC) on CRM for SI-traceable $^{13}C/^{12}C$ isotope ratio measurements, Manfred Gröning (IAEA) on isotope reference materials for environmental applications and Patricia Atkins (SPEX) on challenges in the development of arsenic species reference standards and their use in the analysis of alcoholic apple ciders. Owen Butler (HSL) addressed the development thermal desorption sorbent tubes with semi-volatile organic compounds for subsequent use as proficiency tests or reference material samples. Imma Tolosa (IAEA) spoke on marine sediment reference materials for the determination of trace concentration levels of polycyclic aromatic hydrocarbons and Steven Newmaster (University of Guelph) concluded the session with a presentation about the fundamentals of reference materials in the formation of speciation analyses of biological ingredients.

The conference dinner took place on the evening of the second day at the historic Wasserwerk Hohenzollerndamm. In this beautiful location authentic Berlin meals were served while the discussions around reference materials continued at the different tables. In addition, a prize sponsored by Merck for the best of the 72 posters was awarded to the following participants: Benilda Ebarvia (National Metrology Laboratory Philippines) received the best poster award for her contribution on reference material development for benzoic acid analysis in banana-based Philippine condiments. Second winner was Pranee Phukphatthanachai (BAM) for her work on the quantification of the exact amount of sulphur in organic and inorganic samples, and third winner was Anita Röthke (PTB) with her poster on high accuracy ICP-OES characterization of SI traceable mercury reference standard solutions in support of the European Pharmacopoeia.

The combined sessions for the third conference day addressed the topics around biological and qualitative reference materials as well as commutability of CRMs for clinical analysis with Robert Wielgosz (BIPM) and Christa

Cobbaert (University Leiden) as keynote speakers. Robert Wielgosz addressed the topic of primary reference materials in clinical analyses and the importance to assure a low in-between method variability since results from influence many decisions that are taken in a clinical environment. Christa Cobbaert picked up this topic in her talk about the relevance of commutability of reference materials in laboratory medicine. The session continued with Liesbet Deprez (JRC) who described a new approach for assessing commutability of reference materials for clinical measurements and Claudia Swart (PTB) who showed traceability studies for potential new biomarkers for Alzheimer's Disease. Clay Davis (NIST) presented his research on commutability in proteomics and metabolomics using human tissue reference materials, Alison Whale (LGC) eluded on digital PCR for value assignment of nucleic acid reference materials and Adam Kuszak (NIH) gave an overview on NIH's program for analytical method and reference materials development. Fay Betsou (IBBL) discussed clinical biobanks as providers of biological reference materials and Stephen Ellison (LGC) talk about harmonized stability and homogeneity studies for qualitative reference materials.

In the last session Derek Craston (LGC) was presenting the change in the production of CRMs through recent year. While this topic was historically dominated by NMIs, commercial RM producer are becoming more and more active in that field. Steve Wise concluded the oral presentations with a review on more than 30 years of BERM and provided thoughts about future trends and needs in CRM development.

After the conclusion of the oral presentations a workshop Workshop on Optical Spectroscopy and Quality Assurance in Fluorometry was held at BAM Branch Adlershof.

The huge variety and the very high level of the oral and poster presentation, the discussions and networking in the breaks, over lunch and at dinner as well as the 10 exhibitors from multiple countries contributed together to the huge success of BERM15.

18TH ANNUAL ENBIS CONFERENCE, SPECIAL SESSION ON METROLOGY, NANCY, FRANCE

Francesca Pennecchi // INRIM, Italy

ENBIS (https://enbis.org/) is the European Network for Business and Industrial Statistics, a platform connecting individuals and organizations interested in theoretical developments and practical applications in the field of business and industrial statistics. The mission of ENBIS is to foster and facilitate the application and understanding of statistical methods to the benefit of European business and industry, to provide a forum for the dynamic exchange of ideas and facilitate networking among statistical practitioners, to nurture interactions and professional development of statistical practitioners regionally and internationally, to emphasize multidisciplinary problem solving involving statistics, to link academic teaching and research in statistics with industrial and business practice, and to seek collaborative agreements with related organization. In the range and variety of topics which are of interest for the ENBIS community, an important role is played by 1) the application of statistical methods in measurement science (metrology), and 2) measurement systems in process control, conformance assessment and quality improvement. These themes are particularly handled by the Special Interest Group (SIG) on Measurement Uncertainty (https://enbis.org/about/sig/measurement_uncertainty/index), chaired by Alistair Forbes (UK National Physical Laboratory, NPL) and myself (Italian National Institute for Metrological

Research, INRIM, and CITAC).

Every year, ENBIS organizes an annual Spring Meeting and, traditionally every September, the Annual Conference. The latest annual conference ENBIS-18 was held in Nancy (France), from 2nd to 6th September, 2018 (https://www.enbis.org/activities/events/current/573_ENBIS_18_in_Nancy/). It was hosted by the Laboratory of Mathematics "Institut Elie Cartan" of Lorraine University and took place at the "Ecole des Mines", in Nancy (France). More than 120 presentations were delivered during the conference, with a total of more than 150 participants. Opening and closing keynote speakers were Jean-Yves Tourneret ("A Review of Multiband Image Fusion Methods With a Specific Attention to Bayesian Methods") and Piercesare Secchi ("O2S2 - Object Oriented Spatial Statistics: A Review with Examples"), respectively. The 2018 George Box Medal was awarded to Ron S. Kenett, past President of ENBIS and of the Israel Statistical Association ("The Real Work of Data Science: How to Turn Data into Information, Better Decisions, and Stronger Organizations"). Among the others, several sessions were devoted to Chemometrics, Quality Control, Reliability and Metrology.

Beside contributed sessions, 19 special sessions were also prepared. Among these, I organized a special session on Metrology (https://enbis.org/activities/events/current/573_ENBIS_18_in_Nancy//programmeitem/2681_Special_Session_Metrology), consisting in the following three presentations:

- *Bayesian Models for Evaluation of Risks in Conformity Assessment of Multicomponent Materials or Objects*, Francesca Pennecchi (INRIM, Torino), Ilya Kuselman (Independent Consultant on Metrology, Modiin), Ricardo J. N. B. da Silva (Centro de Química Estrutural, University of Lisboa), Brynn Hibbert (School of Chemistry, Sydney);
- *EMUE: Towards a Comprehensive Set of Examples of Measurement Uncertainty Evaluation to Support Guides and Standards*, Maurice Cox (National Physical Laboratory, NPL);
- *Sequential Design of Experiments to Estimate a Probability of Failure in a Multi-Fidelity Stochastic Simulator*, Séverine Demeyer (Laboratoire National de Métrologie et d'Essais), Rémi Stroh (Laboratoire

National de Métrologie et d'Essais), Nicolas Fischer (Laboratoire National de Métrologie et d'Essais).

The main theme of the session was intended to be the development and the application of statistical methods to metrology in the context of several international projects, i.e., respectively, the IUPAC Project 2016-007-1-500 (2016-2018), the EMPIR Project 17NRM05 EMUE (2018-2021) and the EMRP Project NEW04 (2012-2015). Concerning my presentation, in particular, I showed the main results obtained in the relevant IUPAC Project that was devoted to the modelling of consumer's and producer's risks in the conformity assessment of multicomponent materials, such as medications, alloys, food and clinical samples, or environmental compartments (e.g. ambient air). When multicomponent materials undergo conformity assessment, even if the assessment is successful for each component of the material batch or lot, the total probability of a false decision (total risk), concerning the batch or lot as a whole, might still be significant. Modelling of such scenarios is important for understanding conformity assessment risks in customs control, clinical analysis, pharmaceutical industry, environmental control and other fields. In the IUPAC Project, Bayesian models of total risk evaluation were formulated for both cases of independence and correlation of the involved variables (components concentrations and corresponding test results). In the former case, based on the law of total probability, it was shown that total risks can be evaluated as appropriate combinations of the particular risks (i.e. those related to the particular/separate components). In the latter case, evaluation of the risks required modelling the variables by multivariate prior probability density and likelihood function in order to obtain corresponding multivariate posterior distribution from which the risks could be calculated. In these situations, correlation could have a considerable influence on the seriousness of the risks.

More details about the scientific program and abstracts are available at https://enbis.org/eventdocs/programme_and_abstracts

CITAC
Cooperation on International Traceability in Analytical Chemistry

ANNOUNCEMENTS

4TH INTERNATIONAL SCIENTIFIC & TECHNICAL CONFERENCE "METROLOGY OF PHYSICOCHEMICAL MEASUREMENTS"

17-19 SEPTEMBER 2019, SUZDAL, RUSSIA

The Conference "Metrology of physicochemical measurements" is a good opportunity to meet colleagues active as in physicochemical measurements as in fundamental, applied and legal metrology, to share experiences and to discuss common problems.

ORGANIZERS

All-Russian Research Institute of Physico-technical and Radio-technical measurements (VNIIFTRI), ROSSTANDART.

THE CONFERENCE SUBJECTS

- Electrochemistry: pH and pX measurements
- Spectrometry, chromatography
- Reference materials
- Measurement standards, key and pilot comparisons, traceability
- Dispersed parameters of particles in heterogeneous media, including aerosols and suspensions
- Zeta potential
- Measurements of air ions
- Measurements of properties and parameters of solids
- Physicochemical measurements in applied and legal metrology: ecology and environmental protection, work areas, clean rooms, food, water, health care, atmospheric parameters, and other area related to physicochemical measurements

VENUE

The conference will be held on September 17-19, 2019 in the Hotel Complex "Pushkarskaya Sloboda", located in a historic town - Suzdal, Vladimir Region. Suzdal - fabulously picturesque town. This is an open-air museum, where unique monuments of antiquity are combined with natural splendor. You cannot find many monuments of the Russian history, such as extant intact the old buildings, unique churches and objects of wooden architecture anywhere else. The landscape of Suzdal is the white-stone Kremlin walls along the banks of the river and the cupolas of churches which glint in the sunlight between meadows- reserve. In the city there are 32 active temples and more than 150 monuments of architecture. There are no high-rise buildings and industrial buildings, and the air

is clean and fresh. This is one of the ancient settlements, which has maintained its unique appearance.

TECHNICAL PROGRAM

The conference will include oral and poster presentations. Presented abstracts will be published before the conference in a special issue "Metrology of Physicochemical measurements. Abstracts". After a peer-review, some presentations could be recommended for publication in a reputable scientific journal.

SOCIAL AND CULTURAL PROGRAM

The Organizing committee will offer to participants a special sightseeing tour of Suzdal and the Conference dinner.

Conference working languages: Russian and English.

REGISTRATION:

For more information and registration, please, contact the Scientific Secretary of the Organizing Committee by e-mail: mera@vniiftri.ru

ORGANIZING COMMITTEE:

Conference chair:
Dr. Sergey Donchenko
General Director, VNIIFTRI

Scientific Secretary:
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Deputy Head of Physicochemical and Electrical Measurements Department, VNIIFTRI

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JOINT WORKSHOP OF itENBIS & INRIM MATHEMATICAL AND STATISTICAL METHODS FOR METROLOGY

30-31 MAY 2019, TORINO, ITALY

Recognizing the increasing need of *ad hoc* and innovative mathematical and statistical tools for current and emerging metrological applications in the several areas of the Science of Measurements, the Italian Local Network of the European Network for Business and Industrial Statistics (itENBIS), http://www.enbis.org/about/ln/

itenbis/index, and the Italian National Metrology Institute - Istituto Nazionale di Ricerca Metrologica (INRIM),Ihttps://www.inrim.it/, propose a joint Workshop on Mathematical and Statistical Methods for Metrology.

Highlights of the Workshop include invited speakers, organized and free contribute sessions concerning the main topics of mathematics and statistics for metrological applications.

SESSION TOPICS INCLUDE BUT ARE NOT LIMITED TO:

- Interlaboratory data evaluation
- Uncertainty and measurement quality evaluation
- Regression and inverse models
- High dimensional, dynamic and complex models
- Bayesian models
- Simulated experiments and computational methods
- Machine Learning, artificial intelligence and Big Data analytics
- Statistical engineering
- Design of experiments
- Sampling and sequential design
- Time series analysis
- Conformity assessment, reliability and quality control
- Chemometrics
- Biostatistics

Contributes on analytical chemistry, chemical measurements, associated uncertainty evaluation and quality related issues will be very welcome.

The Workshop venue is INRIM. Instructions on when and how to upload the abstracts, as well as details on registration, travel and accommodation are available at the website of the Workshop.

IMPORTANT DATES

- **18 February 2019** – submission of a title and an extended abstract (max 2 pages) including main references and keynotes
- **15 March 2019** – acceptance notification to the authors
- **3 May 2019** – last date for the payment of the registration fees
- **30-31 May 2019** - Workshop at the INRIM
- In **June** – call for submission of paper to special issue of relevant scientific journals

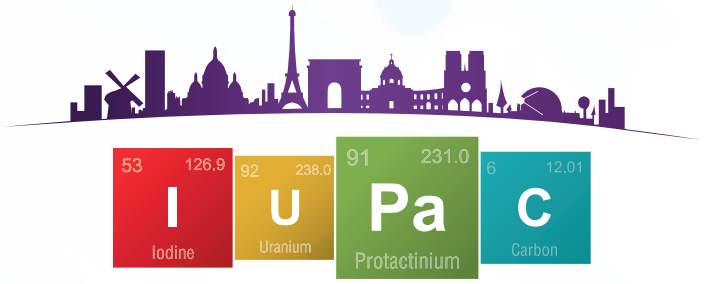
CONTACT PERSONS:

Chairs: Grazia Vicario, Politecnico di Torino (grazia.vicario@polito.it), and Francesca Pennecchi, INRIM (f.pennecchi@inrim.it).

Website: http://www.msmm2019.polito.it/.

Photo by Gian Paolo Scialpi

Under the High Patronage of
Mr Emmanuel MACRON
President of the French Republic

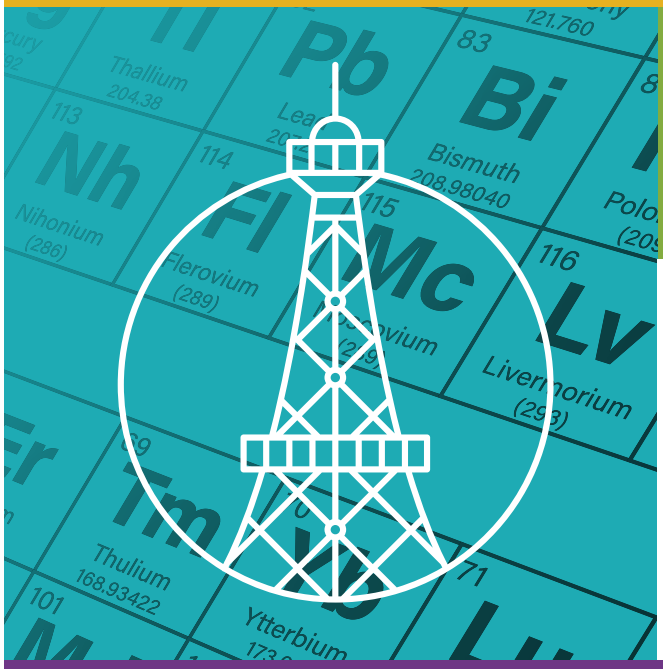


PARIS, FRANCE

50th General Assembly & 47th IUPAC World Chemistry Congress

« Frontiers in Chemistry: Let's create our Future! 100 years with IUPAC »

JULY 5-12 2019



IUPAC will celebrate its Centenary holding its General Assembly and World Congress in Paris, France, along with dedicated sessions and events.

100 IUPAC

IUPAC CENTENARY CELEBRATION

IUPAC PARIS 2019 **www.iupac2019.org**

CITAC
Cooperation on International Traceability in Analytical Chemistry

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ABOUT CITAC

CITAC - Cooperation on International Traceability in Analytical Chemistry - arose out of an international workshop held in association with the Pittsburgh Conference in Atlanta in March 1993. The aim of this workshop was to discuss how analytical activities could be developed to meet the needs of the 21st century, and it identified a wide variety of issues to be addressed to ensure that analytical measurements made in different countries or at different times are comparable. These range from the development of traceable reference materials and methods to the harmonisation of analytical quality practices.

The CITAC Initiative aims to foster collaboration between existing organisation to improve the international comparability of chemical measurement. A Working Group takes matters forward and its initial activities have centred on a few specific high priority activities. The first tasks included the compilation of a directory of certified reference materials under development; preparation of quality system guidelines for the production of reference materials; preparation of a directory of international chemical metrology activities; defining criteria for establishing traceability to the mole; and the preparation of an international guide to quality in analytical chemistry.

Many of these activities are of a strategic nature, laying the ground for the improvement of international analytical measurement. This reflects the added geographical complexities associated with a world-wide organisation, such as greater diversity in culture and in technical approach, and frequently long timescales associated with its activities. Nevertheless, if the full benefits of improved analytical measurement are to be realised internationally, a truly global approach is needed, and there is a clear role for CITAC to play in this respect.

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