



International Union of Pure and Applied Chemistry

Analytical Chemistry Division

TEAMWORK

July 2013

Welcome to TEAMWORK – the magazine of the ACD

The history of TEAMWORK stems from an initiative of Kip Powell (New Zealand) in March 2002 to provide occasional briefings for the IUPAC community on the activities of the Analytical Division. Its production was in response to the sweeping changes that occurred to the structure of IUPAC in the early 2000's; the disbanding of the majority of Commissions and a move to the project system.

The Division now sees the role of TEAMWORK as providing a welcome to the Committee coming towards a General Assembly, and keeping up its tradition of announcing to the wider IUPAC body just what the Analytical Chemists are doing and worrying about.

On behalf of President Camões I give best wishes to Division V as it meets in Istanbul, Turkey at the 47th General Assembly (<http://www.iupac.org/ga/47th>).

Brynn Hibbert, Vice-President

Message from the Division President

Maria Filomena Camões, President, ACD

The present Executive Committee of the IUPAC Analytical Chemistry Division (Maria Filomena Camões (P), Brynn Hibbert (VP), Ales Fajgelj (PP) and Zoltan Mester (S) and Clara Magalhães (SSED)) initiated its term of office at the beginning of the year 2012, for the biennium 2012-2013, after what can be called a transition period that followed the 46th General Assembly, held in August 2011 in S. Juan- Puerto Rico.

Promoted by our colleague Paul de Bièvre, who acted as local organiser, the meeting of the Division Committee took place at the Elzenveld Conference venue, near Antwerp-Belgium, between the 5th and the 7th of February 2012, to discuss activities and plans in the frame of the ACD members' roles and responsibilities.



1: President of Division V, Professor Maria Filomena Camões

Those who had the opportunity to participate may well remember that we had the opportunity to discuss in more detail the state of the art concerning the ongoing Division Projects and some of the overarching IUPAC policies. Triggered by the opportunity and by the expertise and sensitivity gathered in the Group, a strong point of the discussion has been centred on the proposals for the eventual redefinition of the mole and the kg under the light of the constants of Nature. Although there was the stated intention to promote a IUPAC Project on the critical analysis of the mole and the kg issue, involving the various divisions, this proved to be a task of high complexity and has never taken place. Nevertheless the biennium has been the stage for very thorough and enlightening

discussions of the highest scientific level that are far from reaching an end.

The information that would be the guide for the challenges ahead, for the biennium 2012-2013, was updated and disseminated through number 16 of the Division Newsletter, Teamwork. This has been the basis for the Division Report to the Bureau that met a couple of months later, 12-16 April 2012, at Leiden- Netherlands, where there was better understanding of statutes and bylaws, for ensuring a smooth progress along the biennium, basically taking all other steps necessary for the good conduct of the affairs of the Union.

The awareness that there is a modest budget to run, 70% for commitments with approved projects and 30% for operational costs, made us pay convenient attention to the priorities established by the Division members, both through the actions agreed and through a balanced management of the projects that are being submitted. The first priority was reconfirmed to be the Orange Book and its various Chapters, under the overall coordination of Brynn Hibbert. The Division continues to give good consideration to granting support to conferences of relevance to Analytical Chemistry.

We strongly recommend that smaller or bigger reports on projects, conference news and any other important positive outcomes worth knowing about are prepared by the respective chairmen and coordinators and sent for publication in Chemistry International, a IUPAC journal that reaches a wide range of readers.

Half-way through the 2nd year already, after a second Bureau meeting Frankfurt, 19-21 April 2013, and approaching the 47th IUPAC General Assembly, planned for Istanbul- Turkey, 8-15 August 2013, I am starting to write the Division Report to be presented at the Council.

From a long list of points coming to my mind, all of them deserving our thoughts and benefiting from further discussion, I mention just a few key issues on which I would like to have some input from the Division Members on time for inclusion in the Agenda for the Istanbul 47th General Assembly, next August.

At the Bureau all Division Presidents were asked by IUPAC President to select a most representative project of their respective divisions. How would you choose the “best” project? This is no doubt a good question we should keep in mind and pose to ourselves both when we are approving a project application and when we are chairing a project.

What would you like to see contemplated by the Division as part of IUPAC strategic plan? The time has come when discussion on the publication and dissemination system, printed and digital, IUPAC journals and ownership, or not minor points and need decisions. Successive technical problems with IUPAC webpage have made it very difficult, when not totally impossible, to have access to minutes and reports, which certainly slows down the enthusiasm and dedication of members to their tasks.

How to help enforcing the role play of Division members, TM, AM, NR, not only inside the Division, but also on their commitments liaising with the various other committees?

At the end of last year, a nomination and election process was initiated planning for the next biennium 2014-2015. A reinvigorated group, aware of emerging scientific issues, will successfully continue implementing the aspirations of Analytical Chemists, through vivid interchange of ideas within the Division, meeting the objectives of the Union and the needs of Society.

I am looking forward to meeting as many as possible of you in Istanbul, on the 9th and 10th August, for the ACD meetings.

HOT TOPICS

of the Analytical Chemistry Division

Revision of the Orange Book

Brynn Hibbert, Vice-President

The revision of the Orange Book is now in full swing, with eleven chapters being worked on by task groups, backed by projects.

Congratulations to Professor Chai who has submitted his chapter on Radioanalytical methods well ahead of schedule!

The new edition will be a vocabulary of concepts with definitions of terms that are compatible with the format of the Gold Book. All definitions will have been reviewed by PAC/ICTNS and will be compliant with the International Vocabulary of metrology (VIM) and with other IUPAC colour books.

There will be an OB progress meeting on the afternoon of 8th August.

The chapters of the OB are:

Chapter 1: Fundamental concepts and terms (metrology), chemometrics, quality assurance.	Paul De Bièvre.
Brynn Hibbert, (TM)	
Chapter 2: Sampling and sample preparation	Zoltan Mester, (TM)
Chapter 3: Methods of analysis depending on measurements of mass and volume	Maria F. Camões, (TM)
Chapter 4: Separation	Tatyana Maryutina, (AM)/ Attila Felinger (TM)
Chapter 5: Spectroscopic methods of analysis	Yngvar Thomassen, (TM)
Chapter 6: Mass spectrometry	Zoltan Mester (TM)
Chapter 7: Electrochemical methods of analysis	José M. Pingarrón, (TM)
Chapter 8: Radioanalytical methods	Zhifang Chai, Peter Bode (AM)
Chapter 9: Surface analysis	Maria F. Camões, (TM)
Chapter 10: Thermal methods of analysis	Carlos Castro, Maria F. Camões, (TM)
Chapter 11: Immuno- and bio-analytical methods of analysis	Jan Labuda, (TM)

Revision of the SI

As mentioned by the President the Analytical Division has prepared its position on the proposals for revising the definitions of kilogram and mole. Supporting the stance of the CIAAW following the Antwerp Division Committee meeting the following recommendations were agreed.

“In particular we support a definition of the Avogadro *number* that recognises it as a scaling factor of individual entities.

The mole

The ACD **recommends** the following future definition of the mole:

The mole, symbol ‘mol’, is a number of entities equal to 6.022×10^{23} entities exactly

Note 1: The entities must be specified

Note 2: The proposed definition does not require an associated quantity other than ‘1’. However to maintain continuity with the present ISQ, the present quantity ‘amount of substance’ is renamed ‘chemical amount’, and the mole be also recognised as the unit of chemical amount.

Note 3: The International Vocabulary of Metrology (VIM) notes (1.4, Note 3) ‘Number of entities’ can be regarded as a base quantity in any system of quantities.

The ACD **requests** that any decision on redefinition of the mole be deferred until full consideration is given to the interests of the chemical and isotopic measurement communities.

Unit of mass

If the unit of mass is no longer to be tied to the mass of an object (the International Prototype of the kilogram), the ACD proposes that the unit of mass be the gram, symbol 'g'.

Together with the fixed value of the Avogadro number, the dalton could serve to redefine the gram. The ACD **recommends** the following future definition of the gram:

The gram, unit of mass, symbol 'g', is one twelfth (1/12) of the mass of 6.022×10^{23} atoms of ^{12}C in their nuclear ground state."

The debate continues.

Revision of the GUM

VP Hibbert is one IUPAC representative on the Joint Committee for Guides in Metrology Working Group 1 and reports to ICTNS. WG1 is charged with the task of maintaining the Guide to the Expression of Uncertainty in Measurement (GUM) and its supplements. Its current major task is to prepare a new edition to update the guide in the light of advances in understanding of uncertainty since the 1993 edition. A strong presence by chemists and clinical chemists (from IFCC), and from the accreditation body ILAC will hopefully result in a Guide that is clearly relevant to all areas of measurement science. It is hoped a consultation draft will be available in 2014.

Of interest to IUPAC, the WG1 has just responded to a question from CIAAW concerning how to treat uncertainty for the twelve elements whose atomic weights are presently given as a range (e.g. C is [12.0096; 12.0116]). There is a project from the Inorganic Division (2011-040-2-200) and a submitted project proposal from Division V on these issues.

Subcommittee on Solubility and Equilibrium Data

Contributed by Clara Magalhães, Chair of SSED and TM of Division V

One of the major products of the Division is the huge output of the Subcommittee on

Solubility and Equilibrium Data (SSED). Its terms of reference read:

The Subcommittee on Solubility and Equilibrium Data (SSED) coordinates projects in the area of compilation and critical evaluation of published experimental data on the chemical solubility of well defined substances and other equilibrium systems. The SSED also coordinates the dissemination of evaluated solubility data through traditional (journal) and electronic (internet-accessible database) means. The SSED works with the Analytical Chemistry Division and the US National Institute of Standards and Technology (NIST, the Solubility Data Series publisher) in the selection of chemical systems for treatment, encourages the formation of Task Groups to perform compilation and evaluation, and assists Task Groups in carrying out their projects.

The output is published as the "Solubility Data Series". The solubility data project began in 1972 when Stevan Kertes proposed to Commission V.6 to start a project on collecting and evaluating solubility data. The first solubility data project meeting occurred in the Fall of 1974 in Montreal. In 1975 the solubility data project was made a Subcommittee of Commission V.6. This Subcommittee was converted into the Commission V.8 (Solubility Data) of the Analytical Chemistry Division in 1979. Still in 1979 were published the three first volumes of the Solubility Data Series by Pergamon Press. After several changes the Solubility Data Series volumes are now published in the Journal of Physical Chemistry Reference Data that is now publishing the volume 99. With the 2001 IUPAC reform the Subcommittee on Solubility and Equilibrium Data replaced the Solubility Data and the Equilibrium Data Commissions. Besides the compilation and critical evaluation of solubility data the former Commission V.8 and present SSED is also responsible for the organization in even numbered years of the International Symposium on Solubility Phenomena and Related Equilibrium Processes. The first

meeting was held in London, Ontario, Canada, in 1984.

MEETING REPORTS

Contributed by members of the Analytical Division

Central European Workshop

CHEMICAL MEASUREMENT IN 21st CENTURY

National Committee of IUPAC in Slovakia (in cooperation with the Slovak Chemical Society, Eurachem-Slovakia and Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava) organized on 21 to 23 November, 2012, in Bratislava, Slovakia the workshop entitled above. The aim of the workshop was to provide state-of-the-art thinking in concepts and associated terms in chemical measurement for the 21st century. The workshop was also intended to present situation in dissemination and implementation of the new edition of the International Vocabulary of Metrology (VIM 3) in countries of the Central European Region and to share experiences of scientists and researchers in different areas of measurement at universities and research laboratories.



2: Professor Paul De Bièvre at the CENTRAL EUROPEAN WORKSHOP on Chemical Measurement in the 21st Century.

Invited lecturers were Professor Paul De Bièvre from Antwerp, Belgium, Assoc. Prof. David Milde from the Palacky University in Olomouc, Czech Republic, Prof. Sandor Kemény from the University of Technology and Economics in Budapest, Hungary, Prof. Edo Plško from the Comenius University in Bratislava, and Dr. Michal Mariássy a Eng. Maria Valková from the Slovak Institute of Metrology in Bratislava. Numerous workshop participants including PhD students came from the Czech Republic, Poland, Hungary, Rumania and Slovakia.

As a continuation of the workshop, a special seminar under the title Realization of Unit Mole with Respect to its Redefinition was organized at the Slovak Institute of Metrology. Excellent lecturers and working atmosphere of these events contributed significantly to fulfilment of the IUPAC aims.

Jan Labuda, Titular Member

Isranalytica

Isranalytica 2012 Conference and Exhibition David Intercontinental Hotel, Tel-Aviv, Israel, 24–25 January 2012.

The Isranalytica, organized by the Israel Analytical Chemical Society, is the largest analytical conference in Israel and has become one of the largest annual conferences in analytical chemistry in the world. Over the past years, Isranalytica has achieved major success and become the most prestigious analytical chemistry meeting in Israel.

Highlights included plenary lectures by

- Steve Stein (NIST Fellow, MS Data Center, NIST, MD, USA) : ‘Mass spectral reference libraries: an ever-expanding resource for chemical identification’
- Robert J Levis (Department of Chemistry, Temple University, PA, USA) : ‘Imaging molecules using ultra-intense lasers’

- Christine Moore (US FDA, MD, USA) :
'Quality by design and analytical methods: an FDA perspective'
- Guenther Bonn (University of Innsbruck, Austria) with the title 'New enrichment and separation technologies in bioanalysis'

A full report by Prof Bonn can be found in *Bioanalysis* (2012) 4(9), 993–995.

As our NR from Israel, *Daniel Mander* writes *Isranalytica* is a real success. 15 Years ago there was simply nothing and with only a few people very much devoted to advancing analytical chemistry in Israel we have made this as the biggest meeting in chemistry in Israel and one of the largest analytical chemistry meetings in the world.

1st International Congress on Metrology – METROCOL

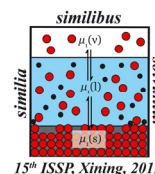
August 13-15, 2012 (Bogotá D.C., Colombia).

Our President, *Maria Filomena Camões* delivered the opening address to this conference which was at the Official Inauguration of the laboratory on Chemical Metrology in Bogotá. The topic of her talk was "Secondary pH measurements and electrical conductivity".



3: President Camões opens conference in Bogota, Colombia

15th International Symposium on Solubility Phenomena and Related Equilibrium Processes



The 15th International Symposium on Solubility Phenomena and Related Equilibrium Processes was held from 23rd to 27th July 2012 at Qinghai Institute of Salt

Lakes, Chinese Academy of Sciences (CAS), Xining, China. This IUPAC-sponsored symposium included a workshop entitled "Solubility and Other Equilibria in Salt Brines." The 11th Annual Meeting of the Subcommittee on Solubility & Equilibrium Data (SSED) of the IUPAC Analytical Chemistry Division met on 21st July, chaired by TM *Clara Magalhães* from Portugal.

Over one hundred participants, including accompanying persons, from 21 countries attended the annual meeting of SSED and the symposium: Australia, Austria, Canada, China, Czech Republic, Denmark, Finland, Germany, Hungary, India, Ireland, Italy, Japan, Nepal, Poland, Portugal, Russia, Slovakia, Ukraine, and USA.

Seven plenary and four invited lectures focused on the six aspects related to solubility phenomena: 1) Equilibria related to solid solutions; 2) Computer assisted equilibrium calculations; 3) Solubility features in ionic liquids; 4) Kinetics of phase transformations; 5) Effects of solute-solvent interactions on solubility phenomena; 6) Solubility phenomena related to brine solution.

Thirty three short communications and fifty three posters were presented during afternoon and morning sessions.



4: Heinz Gamsjäger in his Tang Suit with Clara Magalhães at the banquet

Julia Schmitt was honoured with the 2012 Franzosini award. Three IUPAC poster prizes were given.

Sponsorship was provided by Chinese Academy of Sciences, the National Nature Science Foundation of China, Qinghai Foreign Experts Bureau, Qinghai Institute of Salt Lakes. The Local Organizing Committee financially supported 24 delegates to attend the meeting in various forms.

A banquet in Chinese style was served to participants. During the banquet, a special program was organized to celebrate the 80th birthday of Heinz Gamsjäger. Clara Magalhães chaired the session. Glenn Hefter introduced the curriculum vitae of Heinz Gamsjäger and his achievement in solubility phenomena research and in chairing the SSED of IUPAC. The Local Organizing Committee presented Heinz Gamsjäger a special Chinese birthday gift “Tang suit” and wished him good health and a long life.

**Membership of the Analytical
Division (2012 – 2013)**

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