



## **Report to Council from Division V**

### **(Analytical Chemistry)**

### **General Assembly Busan, August 2015**

#### **I. Highlights of the Division's activities**

The Division of Analytical Chemistry continues to focus its activities on metrology and quality assurance in chemical measurements, compiling critically-evaluated data in solubility and other equilibrium processes, and the terminology of analytical chemistry.

- **Metrology in Chemistry (MiC)**

Division V members represent IUPAC on the Joint Committee on Guides for Metrology (JCGM) (Paul De Bièvre) and its two working groups, WG1, which writes and maintains the Guide to the Expression of Uncertainty in Measurement (GUM) and its Supplements (Brynn Hibbert, until 2015 René Dybkaer), and WG2, which is responsible for the International Vocabulary of Metrology (VIM) (Paul De Bièvre, until 2015 René Dybkaer). IUPAC is mandated to use the terminology and guidance in these documents, and more must be done to both represent chemistry's views to the JCGM, and to explain the approaches and methodology of the VIM and GUM to chemistry. An annotated VIM with more user-friendly language is in preparation. The recent rejection by the member organisations of JCGM of the new edition of the GUM (including IUPAC) is causing the WG1 to re-evaluate its approach. No errors of statistics or logic were discovered, but the IUPAC assessment, for example, reads: (i) The consensus is that the JCGM 100 and 110 are documents that relate only marginally to the work of chemists and chemical engineers, (ii) The documents are written in a manner not easily understood and most impractical; (iii) If the document writers wish to reach the IUPAC audience and have this audience pay attention, the documents need to be revamped to make them relevant to the work of chemists and chemical engineers.

Meanwhile the Division's Technical Report on Metrological Traceability of Chemical Measurement Results has become a *de facto* standard on how to establish traceability to metrological references (P. De Bièvre, R. Dybkaer, A. Fajgelj, D. B. Hibbert. *Pure Appl. Chem.* **83**, 1873, (2011)).

Another recent highlight has been papers on human factors in chemical measurements out of a project from the Interdivisional Working Party for Harmonization of Quality Assurance (I. Kuselman, F. Pennechi, C. Burns, A. Fajgelj, P. de Zorzi. *Pure Appl. Chem.* **84**, 1939 (2012).)

See also Paul De Bièvre report in Teamwork.

- **Critically-evaluated data in solubility and other equilibrium processes (SSED)**

The single most productive enterprise of Division V is the output of the subcommittee on Solubility and Equilibrium Data (SSED) under the present chair Clara Magalhães. This

biennium celebrated the publication of volume 100 of the IUPAC-NIST Solubility Data Series – Rare Earth Metal Fluorides in Water and Aqueous Systems, Part 1. Scandium group (Sc, Y, La), by Tomasz Mioduski, Cezary Gumiński and Dewen Zeng was published in March 2014. During the 47th IUPAC General Assembly in 2013, it was suggested that SSED members should celebrate this important achievement, which is one of the long range IUPAC goals: the international standardization of physical constants. SSED members, supported by a project “One hundred volumes of Plenitude – Celebrating the IUPAC-NIST Solubility Data Series (2014-012-2-500) organised a half-day workshop at the National Fall meeting of the American Chemical Society in 2014. This participation was very fruitful and two publishers – Springer and De Gruyter – showed their interest in using the published data in their on line databases. The SSED held its annual meeting at the 16th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Karlsruhe, Germany, (21 to 26 July, 2014). The need to provide these data in a useful electronic format is looming as an important medium term goal, issues being a publishing model that can deliver as much data as possible to as many scientists at no cost to the recipient, how to maintain and update the database and what added value can be provided electronically.

- Terminology of Analytical Chemistry (the Orange Book)  
Published last in 1997 the Compendium of Analytical Nomenclature, now titled Compendium of Terminology in Analytical Chemistry, is so completely out of date that it needs rewriting. This project has been underway since 2008 and is nearing its end. The original 19 chapters will be reduced to 12 or 13, and many concepts will be re-termed and re-defined. This has caused some concern about how IUPAC treats colour books. Division V has agreed with PAC/ICTNS that all new and redefined terms will be submitted as PAC Recommendations. Then, once approved, the chapters will be re-assembled with existing Orange Book terms, terms from ISO standards, and terms from JCGM (VIM and GUM) and whatever rubric will be added. This procedure will entail considerable editorial work, but we believe this is the best way of ensuring that only properly approved terms will appear in the colour book, and then in the Gold Book. Submitted to PAC is Chapter 2 on Chemometrics. Several other chapters are near to submission. We have had problems with Spectroscopy, but hope to see the Orange book completed in 2016.  
The new edition of the Orange Book could well be the last physical book that is produced in the colour book series. A project (2013-052-1, IUPAC Color Book Data Management) is looking at ways to make the Gold Book independent of its platform and create a modern content management system (CMS). The main benefit of this approach is that terms and their definitions, notes, examples and references can be approved by ICTNS and then instantly be available for the web site, colour book edition or whatever purpose. A demonstration database and CMS will be presented at the General Assembly. The Division believes that PAC should adopt the ISO approach to creation of vocabularies (ISO. Terminology work - Vocabulary - Part 1: Theory and application, 1087-1:2000, Geneva).

## **II. Report of Division activities 2014/15** **(in terms of relevant long term goals)**

- *IUPAC will provide leadership as a worldwide scientific organization that objectively addresses global issues involving the chemical sciences.*

Division V is at the heart of metrological applications in chemistry, together with critically evaluated data. Gold Book and PAC definitions, as chemical terms with the highest authority, have been quoted in courts of law in Australia and Europe. There is no doubt that IUPAC is considered the world authority to determine terminology and nomenclature in the chemical sciences. Through the close association of Division members with NMIs (National Metrology/Masurement Institutes) and standardization bodies (ISO) we ensure chemistry is at the top table in discussions about measurement. We note that the SSED has published in the Journal of Physical and Chemical Reference Data for many years in a collaboration with NIST (National Institute of Science and Technology, the USA national measurement institute). The work of the Interdivisional Working Party for Harmonization of Quality Assurance coordinates with the International Atomic Energy Authority (Vienna). Finally the participation of IUPAC, through members of Division V, in JCGM and its working parties, and the CCQM shows IUPAC leadership in chemical aspects of measurement and units.

- *IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion.*

The products of the Division are the SSED series and our Technical Reports and Recommendations. See list of projects and publications in the next section. In the near future the Orange Book and the Colour Book database will be added. In April 2014 two members of the Division (Brynn Hibbert and Paul De Bièvre) gave invited presentations to a CCQM workshop on the mole as part of the deliberations on the proposed revision of the SI.

- *IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.*

The Division took the opportunity to hold its between-GA meeting in Pecs in Hungary. At the same time as the Division meeting we invited chemists from the local university to join us and observe the workings of the Division. After the formal meeting a one-day workshop was organised on chromatography and separation science, which also included local people.

- *IUPAC will utilize its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.*

At the GA in Istanbul, Division V had one of the largest cohorts of Young Observers (possibly because we started our meeting somewhat earlier than other divisions). As a result we sponsored two projects from Young Observers and their accompanying persons: Mark Kinnan 2013-052-1, IUPAC Color Book Data Management, and Christine Straut 2013-055-2-024 Increasing IUPAC's Social Media Presence. We also note the project 2013-013-1-500 pH Measurement in Seawater, which is, in some way, a legacy of the International Year of Chemistry.

Immediate Past President Maria Filomena Camões, is Coordinator of EuroMaster– “Measurement Science in Chemistry” (MSC), [www.msc-euromaster.eu/](http://www.msc-euromaster.eu/), which is now in its 8th edition and is the result of an initiative of a consortium of 9 European universities. This Masters

course in Analytical Chemistry boasts a 95% employment rate of its graduates. Division V supports this initiative through Professor Camões and offers help and advice on practical matters in analytical chemistry.

- *IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender, and age.*

We have strong representation from NAOs and cover all continents (in which IUPAC has a presence) in our membership. Our immediate Past President is female, as is the Chair of the SSED. There are four females and twelve males among the current officers, TMs and AMs. Our weakness is in the age structure – most are at the senior stages of their careers. We suspect we are not alone in this problem.

### III. Other material

We have decided to reproduce Teamwork, the Division magazine to detail the activities of the Division in the Biennium. The copy is a draft – the completed magazine, Issue 18, will be on the website at <http://www.iupac.org/home/about/members-and-committees/divisions/v/teamwork.html> for the Busan GA. Note that some tabular material that will be in Teamwork is transferred to part IV of this report.

## TEAMWORK

### the Magazine of the ACD - July 2015

### Welcome to Teamwork 2015

Teamwork is the periodically published product of the Analytical Chemistry Division since 2002. Preparing this magazine, the Division informs its main activities and key products coming to the IUPAC General Assembly, and, at the same time, announce what the Analytical Chemists are doing and thinking about. Further information can be found on the IUPAC Analytical Chemistry Division website: [http://www.iupac.org/nc/home/about/members-and-committees/db/division-committee.html?tx\\_wfqbe\\_pi1\[title\]=Analytical%20Chemistry%20Division&tx\\_wfqbe\\_pi1\[publicid\]=500](http://www.iupac.org/nc/home/about/members-and-committees/db/division-committee.html?tx_wfqbe_pi1[title]=Analytical%20Chemistry%20Division&tx_wfqbe_pi1[publicid]=500)

On behalf of the Division V President *Brynn Hibbert*, I would like to express best wishes to the Division meeting at the 48th IUPAC General Assembly in Busan, Korea.

Jan Labuda, the Vice-President of the Division

This issue of the Teamwork includes:

1. Message from David Brynn Hibbert, the President of ACD
2. Officers and Division meeting in Pecs, Hungary, 27 and 28 March, 2014
3. Membership of committees
4. Revision of the Orange Book
5. News from the revision of IUPAC Colour Books
6. JCGM report
7. Update on SI redefinition
8. Cooperation with EuChemS and ECTN
9. Report of the Subcommittee on Solubility and Equilibrium Data
10. Articles in Chemistry International
11. IUPAC Recommendations and Technical Reports
12. Projects covered by the Division

13. International Workshop on Determining Antioxidants as Reactive Species Scavengers, Istanbul, 27 to 28 October, 2014
14. Membership of the ACD (2014 – 2015)

## **Message from David Brynn Hibbert, the President of ACD**

My I add my welcome to that of the editor to this edition of Teamwork. The Analytical Division of IUPAC continues to be active in the fields of critically-evaluated data (through the energetic work of Clara Magalhães and the SSED), quality assurance and metrology in chemistry, pH (our newest subcommittee) and the on-going revision of the Orange Book. We have continued, during the changing of the guard (or some of them) at Headquarters, to support Analytical Chemistry and to contribute to the work of IUPAC through membership of the Bureau, ICTNS, CPCDS and other committees and bodies, internal and external to IUPAC. See later in this report for a full report of our representation.

Our involvement with the Joint Committee for Guides on Metrology and its working groups is perhaps seeing the end of an era, with the recently announced retirement of René Dybkaer. His knowledge of metrology and terminology is legendary and his “An Ontology on Property for physical, chemical, and biological systems” ([www.ontology.iupac.org](http://www.ontology.iupac.org)) has provided the logical framework for many publications in this field. Reports from our representative Paul De Bièvre will be found elsewhere in this newsletter.

### *Officers and Division meeting in Pecs, Hungary, 27 and 28 March, 2014*

Our off-year (between General Assemblies) Division meeting was held in March 2014 in Pécs in Hungary at the Hungarian Academy of Science. This amazingly embellished building in the Italian Renaissance style had been built by one of the wealthiest merchants in Pécs, György Vasváry in 1884 and provided a magnificent home for our meeting. I was honoured to stay in the President’s suite, which had furniture and décor very fitting to our endeavours. Most officers and TMs attended (Prof. D. Brynn Hibbert, Prof. Jan Labuda, Dr. Zoltán Mester, Prof. Maria F. Camões, Prof. Christo Balarew, Prof. Attila Felinger, Prof. M. Clara F. Magalhães, Prof. Yi Chen, Prof. Heli Sirén, Prof. Tatyana Maryutina) and the NR from Belgium Prof. Paul De Bièvre also was present. During our meeting we had visits from chemists from the local university.

The meeting discussed organisation of the Division, reviewed projects and received reports from our representatives on committees. There was a long discussion on the revision of the Orange Book, and a following seminar on Analytical Separation methods at which the draft of Chapter 4 was discussed and planned.

At the 2013 General Assembly in Istanbul the Division became a sponsor of a project to consider the IUPAC position on the proposals for revision of the SI (A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities, # 2013-048-1). Our representative Zoltan Mester gave a report on the initial work of the task



group. Paul De Bièvre and Brynn Hibbert had been invited to give presentations to a CCQM workshop at the BIPM on the redefinition of the mole in April. The need for IUPAC to advise on the quantity amount of substance and its unit mole has been recognised by the CPGM. To what extent our voice will be heard remains to be seen.

The minutes can be accessed at the web page

<https://www.dropbox.com/s/p4vbu36nndp3s2x/Attendance%20sheet%20Division%20Committee%20Meeting%202014%20Pecs.docx>



Division meeting 27 and 28 March 2014, Villa Vasváry, Pécs, Hungary. Left to right: Prof. Attila Felinger, Prof. Maria F. Camões. Prof. Tatyana Maryutina, Prof. Heli Sirén, Prof. Yi Chen, Prof D. Brynn Hibbert, Prof. Paul De Bièvre, Dr. Zoltán Mester, Prof. M. Clara F. Magalhães, Prof. Christo Balarew, Prof. Jan Labuda.

## Membership of committees

The Division has concerns about the organisational structure for the appointment of IUPAC representative to outside bodies. At present there is no clear process to approve and fund these very important roles. A list of ACD members on internal and external committees is given below.

Body/ Committee/ Organisation	Membership
Internal	

Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)	Brynn Hibbert
Committee on Chemical Education (CCE)	Yi Chen
Committee on Chemical Industry (COCI)	Christo Balarew
Committee on Publications and Cheminformatics Data Standards (CPCDS)	Brynn Hibbert
Pure and Applied Chemistry (PAC) Editorial Advisory Board	Nelson Torto
External	
International Committee on Weights and Measures/Consultative Committee on the Amount of Substance (CIPM/CCQM)	Aleš Fajgelj
ISO-Committee on Reference Materials (ISO/REMCO)	Aleš Fajgelj
Joint Committee for Guides in Metrology (JCGM)	Paul De Bièvre
Joint Committee for Guides in Metrology Working Group1 (JCGM WG1)	Brynn Hibbert and René Dybkaer
Joint Committee for Guides in Metrology Working Group 2 (JCGM WG2)	Paul De Bièvre and René Dybkaer
Inter-Agency Meeting (IAM)	Zoltán Mester
EUCHEMS	Filomena Camões and Jan Labuda
African analytical network	Nelson Torto
CITAC	Ilya Kuselman/ Aleš Fajgelj

I am looking forward to meeting as many of you as possible for the ACD meetings at the GA in Busan, Korea, on the 8<sup>th</sup> and 9<sup>th</sup> August.

David Brynn Hibbert, President

## HOT TOPICS

### *Revision of the Orange Book*

Brynn Hibbert

The revision of the Orange Book is, hopefully, in its latter stages, with twelve chapters being worked on by task groups, some backed by projects.

The new edition will be titled “Compendium of Terminology in Analytical Chemistry” and will be a vocabulary of concepts with definitions of terms that are compatible with the Gold Book.

The present status of chapters of the OB is:



<b>Chapter</b>	<b>Editor</b>	<b>Comments</b>
Chapter 1: Fundamental concepts and terms (metrology), quality assurance.	Paul De Bièvre	Draft under discussion
Chapter 1a. Chemometrics terms	Brynn Hibbert	PAC Recommendations about to be submitted
Chapter 2: Sampling and sample preparation	Janusz Pawliszyn	PAC Recommendations about to be submitted
Chapter 3: Methods of analysis depending on measurements of mass and volume	Maria F. Camões, (TM)	Awaiting draft
Chapter 4: Separation	Tatyana Maryutina, (AM)/ Attila Felinger (TM)	Revised draft under discussion.
Chapter 5: Spectroscopic methods of analysis	Derek Craston (LGC)	looking at possibilities
Chapter 6: Mass spectrometry	Zoltan Mester (TM)	Draft under discussion
Chapter 7: Electrochemical methods of analysis	José M. Pingarrón, (TM)	Draft under discussion
Chapter 8: Radioanalytical methods	Zhifang Chai, Peter Bode (AM)	Two versions available. PB to prepare consolidated draft.
Chapter 9: Surface analysis	Jim McQuillan (Jim is a late comer to this chapter and kindly stepped in after the untimely death of Luisa Abrantes)	Awaiting draft
Chapter 10: Thermal methods of analysis	Carlos Castro	Awaiting draft
Chapter 11: Immuno- and bio-analytical methods of analysis	Jan Labuda, (TM)	Third draft under discussion.

It can be seen that about half the chapters are in a reasonably advanced state. The editor (DBH) will help prepare PAC Recommendations for new terms and definitions (not including ones unchanged from the present OB, JCGM and ISO Standards ), and when these have gone through the PAC review process, will be reintegrated into the OB. Because of the size of the draft chapters and two-paced nature of the appearance of drafts, we might contemplate publishing the OB in two volumes.

It is also expected that going through PAC recommendations will facilitate uptake into the new electronic Gold Book, being worked on by project “IUPAC Color Book Data Management” <http://www.iupac.org/project/2013-052-1-024>.

### *News from the revision of IUPAC Colour Books*

Paul De Bièvre, the IUPAC Representative to the JCGM (Joint Committee on Guides for Metrology)

We (ORANGE BOOK, Chapter 1 responsables) proceeded by just borrowing from VIM all the concept definitions we deemed useful or necessary for Analytical Chemistry, thus automatically keeping the format etc, leaving the ultimate choice of format for later: that is to be decided on the "OB level".

We thereby observed - and followed the logic - that VIM and GUM are the ultimate base documents for all communication in science and technology, and unanimously approved after formal reviewing and voting procedures by eight international organizations: BIPM, IEC, IFCC (yes!), ILAC, ISO (yes!), IUPAC (yes!), IUPAP, OIML; that has made VIM and GUM into some sort of binding "documents" for all these organizations, and, in fact worldwide, for the fields concerned.

ISO Guides and Standards (including ISO International Standard ISO 10241-1 - as other Standards which chemists are simply unaware of (sic!) - are looked at by 2/3 of the world population as "lighthouses" or "references" for intercontinental understanding (as the name and membership of ISO implies), not just "international" i.e. Western world. We do not expect that a small field (chemistry / IUPAC) could convince the other seven members of the approving "Club of Eight" to change the ground rules for defining concepts and the way to write them. That is particularly true for the SILVER BOOK 1 (1995), approved as an IFCC-IUPAC undertaking, and now being reviewed to be approved by IFCC and IUPAC as "SILVER BOOK 2". Further to the previous point: in view of the importance to have a formal reference document in heavily regulated Clinical Analysis and Laboratory Medicine, any change has the potential to cause big problems (changes in regulations are not that easy to perform).

As far as we can perceive, in the International Vocabulary of Nominal Properties (VIN), now on its way, the same principles have been used as in VIM (and GUM).

Further: the substitution principle is a very logical and compulsory principle in the definitions we agree.

Hence, this problem of "standardization" (a field of ISO "par excellence") does concern all of us and has the potential of wide ramifications, e.g., in the revision of other Color Books such as the (badly needed) Gold Book ...

We urge deep reflecting on the above and discourage any definition deviating from the above guiding principles before all of the consequences of choices have been carefully reviewed, and the "way out of chaos" in terminology has been carefully established.

## **JCGM report**

Paul De Bièvre, the IUPAC Representative to the JCGM (Joint Committee on Guides for Metrology)

1. The 2014 JCGM meeting was held on 2014-12-03 at the location of BIPM, one of the JCGM members, currently chairing JCGM for the period 2014-2016.
2. The JCGM heard reports from its WG1 (on the GUM) and its WG2 (on the VIM).
3. It was decided to have a closer look at the re-written Chapters 1, 2 and 3 of the SI Brochure (in the light of the ongoing revision of the SI units) in the light of the March 2015 deadline to submit comments to the CCU.
4. A small WG on "Dimensionless Quantities" has been set up at the instruction of Prof. J. Ullrich (the new President CCU) headed by J. Stenger (PTB); meeting in Feb 2015.

5. We reported that there was no news on the IFCC - IUPAC joint VIN (presumably still in the IUPAC - IFCC evaluation stage). I have been asked to enquire about this.
6. A report was heard from ISO - REMCO on RMs for "qualitative analysis".
7. The current Secretary of the JCGM, Dr. C. Thomas, will resign from her office at BIPM (and of JCGM Secretariat) in June 2015. She will be succeeded by Dr. R. Sitton (BIPM).
8. The next JCGM meeting is on 2015-12-02
9. An increasing use of the GUM in the chemical community was reported. Idem for the VIM.
10. Another discussion took place about the choice between "giving guidance to the lab floor" vs "inputting from the lab floor into the VIM"
11. A message was given to the ISO Delegate, Mrs. Mercè Ferrrés, about ISO 5725 being in bad need of revision.
12. Increasing interest and use of GUM and VIM in the chemical community was reported.
13. The revision of the IUPAC ORANGE BOOK was announced and the achievement of the revised SILVER BOOK 2 communicated to JCGM.
14. Examples of MTr Chains of measurement data obtained on biological materials are very much wanted (dixit IFCC President Beastall)!

## Update on SI redefinition

Zoltan Mester

Presentations to CCQM (10<sup>th</sup> April, 2014) can be found on the website:

<https://www.dropbox.com/s/51t4n1zol91y9lm/CONCERNS%20and%20ISSUES%20in%20the%20re-definition%20of%20the%20mole%20copy%20.ppt>

<https://www.dropbox.com/s/hcnwaddb3vesgxz/Presentation2CCQM.pptx>

## Cooperation with EuCheMS and ECTN

Maria Filomena Camões, EuroMaster Coordinator

The EuroMaster programme "Measurement Science in Chemistry" (MSC), [www.msc-euromaster.eu/](http://www.msc-euromaster.eu/), is now at its 8<sup>th</sup> edition and is the result of an initiative of a consortium of 9 European universities, University of Lisbon- P, University Claude Bernard Lyon 1- F, University of Warsaw- PL, University Maria Curie-Skłodowska- PL, University Adam Mickiewicz- PL, University of Tartu- EE, University of Oulu- Fin, Free University of Brussels-B, University of Maribor- SI, and of the JRC-IRMM. It has been awarded the Eurolabel<sup>®</sup> by ECTN for the 2<sup>nd</sup> consecutive period, since 2007. The MSC EuroMaster is associated with the Master course in Analytical Chemistry at the students' home universities. Between the 1<sup>st</sup> and the 2<sup>nd</sup> year the students benefit from a two week intensive course, the famous Summer School where, in an international environment, real life challenges such as running a laboratory under the requirements of the ISO/EN 17025, add competences and skills that make the difference.

A meaningful employability rate of 95%, very different from the general picture of high unemployment, is the situation for the 280 students who have graduated since 2008. Celebrating success (see Photo), 46 students participated in the 3<sup>rd</sup> graduation ceremony, that took place

recently (12<sup>th</sup> December 2014) in Brussels at the Royal Flemish Academy of Belgium for Science and the Arts. Profiting from this opportunity a workshop on “Employability of Chemistry Graduates” was organized. The various perspectives of both trainers and employers were presented and debated. The invited speakers were Professors Reiner Salzer (DAC-EuCheMS), David Cole-Hamilton, (EuCheMS), Francesco De Angelis (ECTN) and Dr. Sophie Wilmet (CEFIC).

A protocol was signed by MSC, ECTN and EuCheMS stressing the active cooperation observed along the past years and strengthening new forms of future collaboration.



## **Reports from Subcommittees**

### *Subcommittee on Solubility and Equilibrium Data*

Clara M. Magalhães, Chair of SSED and TM of Division V

The year of 2014 was very special for the members of the SSED. The first part of the Volume 100 of the IUPAC-NIST Solubility Data Series – Rare Earth Metal Fluorides in Water and Aqueous Systems, Part 1. Scandium group (Sc, Y, La), by Tomasz Mioduski, Cezary Gumiński and Dewen Zeng was published in March 2014 in the volume 43 (number 1) of the Journal of Physical and Chemical Reference Data. The Part 2, Rare Earth Metal Fluorides in Water and Aqueous Systems, Light Lanthanides (Ce-Eu), is just being published in the volume 44 (number 1) by the same authors.

Once the publication of one hundred volumes inside a very specialized scientific subject is a very rare achievement, it was considered important to celebrate it in a special way. During the 47th IUPAC General Assembly in 2013, David Martinsen and René Deplanque suggested that SSED members should celebrate this important achievement, which is one of the long range IUPAC goals: the international standardization of physical constants. It was suggested that SSED members participate in the National Fall meeting of the American Chemical Society in 2014,

once this is a meeting with a large participation of chemists, not only from the United States of America but also from all around the world. The project “One hundred volumes of Plenitude – Celebrating the IUPAC-NIST Solubility Data Series (project number 2014-012-2-500) was submitted and approved.

248th ACS National Meeting, San Francisco, CA – Session: The IUPAC Solubility Data Series: 100 volumes of Solubility Data Online – Wednesday, 13 August, 2014

The members of SSED were responsible for the half day session “The IUPAC Solubility Data Series: 100 volumes of Solubility Data Online” that occurred on the 13th August 2014 in San Francisco, California. This participation was very fruitful and two publishers – Springer and De Gruyter – showed their interest in using the published data in their on line databases.

The following lectures were presented in the session:

- Mark Salomon (SSED member and IUPAC Editor-in-Chief of the Solubility Data Series): Objectives of the Solubility Data Series
- Allan H. Harvey and Donald R. Burgess (Co-Editors-in-Chief of the Journal of Physical and Chemical Reference Data): NIST Standard Reference Data and the Solubility Data Series
- Stuart Chalk (University of North Florida): REST API for the IUPAC Solubility Data Series: A "Skunkworks" project
- Zdeněk Wagner, Johan Jacquemin and Magdalena Bendová (SSED and members of the IUPAC project “Database on solubility and liquid-liquid equilibria of binary mixture of (ionic liquid and molecular solvent)“): Database on ionic liquids solubilities in molecular solvents: Progress and prospects
- Glenn Hefter (SSED member and Chair of the Stability Constants subcommittee): Critical Evaluation of Stability Constant Data by IUPAC
- William E. Acree Jr. (SSED member): Models to evaluate experimental solubility data for crystalline nonelectrolyte solutes in organic mono-solvents and solvent mixtures
- Earle Waghorne (Secretary of SSED): Thermodynamics of electrolyte solubility in mixed solvents: Silver halides



- M. Clara F. Magalhães and Justin Salminen (Chair and members of SSED): Possible contributions from the Solubility Data Project for arsenic and carbon dioxide environmental impacts mitigation

**Presenters of the oral communications in The IUPAC Solubility Data Series: 100 volumes of Solubility Data Online. Back row from left to right: William Acree, Mark Salomon, Stuart Chalk, Allan Harvey; Front row from left to the right Glenn Hefter, Clara Magalhães, Johan Jacquemin, and Earle Waghorne**

A full report by Clara Magalhães



can be found in the ACS Chemical Information Bulletin (2014) 66(4), pp. 47-50 that can be viewed from the web address: [http://bulletin.acscinf.org/PDFs/CIB\\_66-4.pdf](http://bulletin.acscinf.org/PDFs/CIB_66-4.pdf)

16th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Karlsruhe, Germany, 21 to 26 July, 2014

The 16th International Symposium on Solubility Phenomena and Related Equilibrium Processes was organized by the Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal (KIT-INE), Karlsruhe Germany. This IUPAC-sponsored symposium included a workshop entitled “Solubility and Speciation in Nuclear Waste Disposal”. The 13th Annual meeting of the Subcommittee on Solubility & Equilibrium Data (SSED) of the IUPAC Analytical Chemistry Division met on the 20th July 2014, chaired by TM Clara Magalhães from Portugal.



More than one hundred participants from 24 countries (Australia, Austria, Bulgaria, Canada, China, Czech Republic, Denmark, Finland, France, Germany, Hungary, Ireland, Israel, Italy, Japan, Poland, Portugal, Russia, Serbia, South Korea, Spain, Sweden, Switzerland and USA) representing four continents attended the meeting and the workshop. Five plenary and two invited lectures focused on the seven specific topics related to solubility: 1. Investigation and analytics of aqueous solutions; 2. Aqueous solutions at high ionic strength; 3. Kinetics of phase transformations; 4. Molten salts and ionic liquids; 5. Effects of solute-solvent interactions on solubility phenomena; 6. Solubility phenomena in technical and industrial applications; 7. Computer assisted equilibrium calculations and related thermodynamic databases. Forty short communications and fifty posters were also presented during afternoon and morning sessions.

Franzosini Award: Magdalena Bendová, Institute of Chemical Process Fundamentals Prague, Czech Republic, and S. Gadzuric, University Novi Sad, Serbia were the recipients of the 2014 Franzosini Award.

Three poster prizes were also given.

Sponsorship was provided by IUPAC, the NUSAFE program of HGF (Germany), and the BASF company.

During the conference banquet was celebrated the 80th birthday of Christo Balarew. Clara Magalhães chaired the session and Stefka Tepavitcharova introduced the curriculum vitae of Christo Balarew focusing his achievements in IUPAC and his research in the field of solubility.



The book “The Experimental Determination of Solubilities” edited by G. T. Hefter and R. P. T. Tomkins was offered him as a birthday gift.



*13th Annual meeting of the Subcommittee on Solubility and Equilibrium Data on the 20th July 2014, in Karlsruhe, Germany*

## **Projects**

### *Recently completed projects*

Within last two years, the following projects have recently been completed:

1. 2008-002-1-500, B. Hibbert chair
2. 2014-006-1-500, W. E. Acree chair

### *Running projects*

The Division has about 35 running projects, including those that belong to the Subcommittee on Solubility and Equilibrium Data, the Interdivisional Working Party for Harmonization of Quality Assurance and interdivisional projects. At present, the division focuses its human and financial resources on the updating of the Orange Book. The division feels that the division projects are running reasonably well.

### *New projects*

The following projects have recently been approved:

1. 2014-012-2-500, C. Magalhaes chair
2. 2014-027-1-500, I. Kuselman chair

## **Meeting Reports**

International Workshop on Determining Antioxidants as Reactive Species Scavengers, Istanbul, 27 to 28 October, 2014

The workshop was organized jointly by the Istanbul University and the Analytical Chemistry Division of IUPAC with Prof. Dr. Reşat APAK (Istanbul University), the workshop chairman, and Assist. Prof. S. Esin ÇELİK (Istanbul University), the workshop secretary. Altogether 95 participants attended the workshop. Book of Abstracts is online published in the workshop website: <http://antioxidantworkshop2014.istanbul.edu.tr/>

Plenary speakers were:

- Prof. Dr. Antony Calokerinos (National and Kapodistrian University of Athens): “Luminescent methods for the evaluation of antioxidant activity of olive oil and other natural products”
- Prof. Dr. Sheal Gorinstein (The Hebrew University – Hadassah Medical School): “Nutritional and Pharmaceutical Applications of Bioactive Compounds of Some Edible Berries and Tropical Fruits”
- Prof. Dr. Marcela Segundo (University of Porto): “Automatic flow based methods to evaluate the scavenging activity of antioxidants against ROS and RNS”
- Prof. Dr. İlhami Gülçin (Atatürk University) “Antioxidant compounds: Structure-carbonic anhydrase isoenzymes inhibition studies”
- Prof. Dr. Reşat Apak (Istanbul University): “Comparative evaluation of selected antioxidant capacity/activity assays with special reference to CUPRAC, CERAC and ferricyanide methods”

Keynote Speakers and Lectures were given by:

- Prof. Dr. Vural Gökmen (Hacettepe University): “Antioxidants Bound to Insoluble Food Matrix: Their Measurement, Regeneration Behavior, and Nutritional Relevance”
- Prof. Dr. Cevdet Demir (Uludağ University): “CHROMAC Antioxidant Capacity Method: Principles and Applications”
- Assoc. Prof. Esra Çapanoğlu Güven (Istanbul Technical University): “Evaluating the in vitro bioaccessibility of phenolics and antioxidant activity during consumption of dried fruits with nuts”.



Family photo of the International Workshop on Determining Antioxidants as Reactive Species Scavengers in Istanbul University Congress & Cultural Center.



Prof. Apak, Workshop chairman, presented copper plates to the plenary speakers at gala dinner held in Istanbul University Baltalimanı Social Facility.

#### IV. Tabular material.

##### Membership of the ACD (2014 - 2015)

Officers	
President of the Division	Brynn Hibbert
Vice President	Jan Labuda
Secretary	Zoltán Mester
Past President	Filomena Camões
Titular Members	
	Christo Balarew,
	Yi Chen
	Attila Felinger,
	Kim, Hasuck
	M. Clara Magalhães,
	Heli Sirén
Associate Members	
	Resat Apak,
	Peter Bode,
	Derek Craston,
	Yook Heng Lee,
	Tatyana Maryutina,
	Nelson Torto
National Representatives	
	Othman Othman Chande
	Laurence Charles
	Paul De Bièvre
	Marcos Eberlin
	Ales Fajgelj
	Kate Grudpan
	Javed Hanif
	Daniel Mandler
	Predrag Novak
	David Shaw

#### Publications

Note publications dated 2013 that were not included in the last report are given here.

*Articles in Chemistry International*

- D. Brynn Hibbert, Twitter in Chemical Education, and IUPAC  
2015, Vol. 37, Issue 3, p. 10–11
- Marcus Altmaier, Solubility Phenomena and Related Equilibrium Processes  
2015, Vol. 37, Issue 2, pp. 30-31
- David Shaw, 100 volumes of IUPAC's Solubility Data Series  
2015, Vol. 37, Issue 1, p. 30
- Kipton J. Powell, Paul L. Brown, Robert H. Byrne, Tamás Gajda, Glenn Hefter, Ann-Kathrin Leuz, Staffan Sjöberg and Hans Wanner, Chemical Speciation of Environmentally Significant Metals, 2015, Vol.37, Issue 1, pp. 15-19
- William E. Acree, Solubility of Nonsteroidal Anti-inflammatory Drugs (NSAIDs) in Neat Organic Solvents and Organic Solvent Mixtures  
2014, Vol. 36, Issue 5, p. 21
- Tomasz Mioduski, Cezary Gumiński and Dewen Zeng, Rare Earth Metal Fluorides in Water and Aqueous Systems, 2014, Vol. 36, Issue 4, p. 20
- Marian Góral, David G. Shaw, Andrzej Maczyński, Barbara Wiśniewska-Goćłowska, and Pawel Oracz, Alcohols + hydrocarbons + water, 2014, Vol. 36, Issue 4, p. 18
- Paul De Bièvre, Metrological Traceability of Measurement Results in Chemistry: basic concepts required for intercontinental communication of results,  
2014, Vol. 36, Issue 4, pp. 16–17
- Paul De Bièvre, Chemistry Conference for Young Scientists  
2014, Vol. 36, Issue 4, p. 32
- Analytical Chemistry (13-15 January 2015, Tel Aviv, Israel)  
2014, Vol. 36, Issue 4, p. 34
- Maria F. Camões, pH Measurement in Seawater  
2014, Vol. 36, Issue 3, p. 13
- Solubility Phenomena, 2014, Vol.36, Issue 2, p. 33
- Roberto Marquardt et al., On the New Definition of the Mole  
2013, Vol. 35, Issue 6, p. 29
- Dewen Zeng, Solubility Phenomena, 2013, Vol. 35, Issue 3, pp.32-33

*IUPAC Recommendations and Technical Reports published in Pure and Applied Chemistry*

- Kipton J. Powell, Paul L. Brown, Robert H. Byrne, Tamás Gajda, Glenn Hefter, Ann-Kathrin Leuz, Staffan Sjöberg and Hans Wanner  
Chemical speciation of environmentally significant metals with inorganic ligands. Part 5: The  $\text{Zn}^{2+} + \text{OH}^-$ ,  $\text{Cl}^-$ ,  $\text{CO}_3^{2-}$ ,  $\text{SO}_4^{2-}$ , and  $\text{PO}_4^{3-}$  systems (IUPAC Technical Report)

2013, Vol. 85, Issue 12, pp. 2249-2311

Ute Resch-Genger and Knut Rurack

Determination of the photoluminescence quantum yield of dilute dye solutions (IUPAC Technical Report)

2013, Vol. 85, Issue 10, pp. 2005-2013

Kermit K. Murray, Robert K. Boyd, Marcos N. Eberlin, G. John Langley, Liang Li and Yasuhide Naito

Definitions of terms relating to mass spectrometry (IUPAC Recommendations 2013)

2013, Vol. 85, Issue 7, pp. 1515-1609

Jörg Enderlein

Fluorescence correlation spectroscopy (IUPAC Technical Report)

2013, Vol. 85, Issue 5, pp. 999-1016

Reşat Apak, Shela Gorinstein, Volker Böhm, Karen M. Schaich, Mustafa Özyürek and Kubilay Güçlü

Methods of measurement and evaluation of natural antioxidant capacity/activity (IUPAC Technical Report)

2013, Vol. 85, Issue 5, pp. 957-998

Antonio Doménech-Carbó, Jan Labuda and Fritz Scholz

Electroanalytical chemistry for the analysis of solids: Characterization and classification (IUPAC Technical Report)

2013, Vol. 85, Issue 3, pp. 609-631

Marcel Ameloot, Martin vandeVen, A. Ulises Acuña and Bernard Valeur

Fluorescence anisotropy measurements in solution: Methods and reference materials (IUPAC Technical Report)

2013, Vol. 85, Issue 3, pp. 589-608

## Current Active Projects

Project	Title	Series/ subcommittee
2005-035-2-500 Belli	Trace elements analysis: role of grain size distribution in solid reference materials	
2006-034-1-500 Clever	The solubility of oxygen in all solvents	SSED
2007-047-1-500 Sazonov	Solubility data related to industrial processes. Nitriles C+3: binary and multicomponent systems	SSED
2008-025-1-500 Filella	Humic-metal binding constants database	SSED
2009-006-1-500 Ellison	Experimental Requirements for Single-Laboratory Validation	IWHQA
2010-030-1-500 Chai	Radioanalytical Chemistry - Revision	OB



*IUPAC Analytical Chemistry Division*

	of the Orange Book CHAPTER 16	
2010-052-1-500 Pingarron	Electroanalytical Chemistry - The Revision of the Orange Book CHAPTER 7	OB
2010-061-2-500 Malek	Using process mapping to support (analytical) laboratory processes	IWPHQA
2011-031-1-500 Voigt	Solubility of Lithium Sulfate in Aqueous Solutions	SSED
2011-043-1-500 Shaw	Solubility data related to Industrial Processes. Solubility data in ternary systems containing water, alcohol, and hydrocarbon	SSED
2011-046-1-500 Maryutina	Separation - Revision of the Orange Book CHAPTER 4	OB
2011-047-1-500 Labuda	Recent advances in bioanalytical chemistry: characterization and classification - Revision to the Orange Book CHAPTER 11	OB
2011-063-1-500 Pawliszyn	Sampling and sampling preparation - Revision of Orange Book CHAPTER 2	OB
2011-065-3-500 Bendova	Database on liquid-liquid equilibria of binary mixtures of (ionic liquids and molecular compounds)	SSED
2012-004-1-500 Gamsjager	Solubility of lead carbonates	SSED
2012-007-1-500 De Bievre	Metrology - IUPAC Orange book CHAPTER 1	OB
2012-008-1-500 Hefter	Critical Evaluation of Thermodynamic Data of Sulfate Complexes in Solution	SSED
2012-021-1-500 Kuselman	Classification and modeling human errors contributing to measurement uncertainty of chemical analytical test results	IWPHQA
2012-022-1-500 Eysseltova	Solubility in Systems with Lithium and/or Sodium Nitrates Part 2 - Sodium Nitrates	SSED
2012-030-1-500 Guminski	Rare Earth Metal (Sc, Y, Lanthanoids) Fluorides in Water and Aqueous Systems	SSED
2012-031-1-500 Shaw	Modernizing the website of the Subcommittee on Solubility and Equilibrium Data	SSED
2013-013-1-500 Camoes	pH Measurement in Seawater	pH
2013-015-1-500 Apak	Methods to evaluate the scavenging activity of antioxidants toward reactive oxygen and nitrogen species (ROS/RNS)	

2013-025-2-500 Westwood	Methods for the SI Value Assignment of the Purity of Organic Compounds for use as Primary Reference Materials and Calibrators	IWPHQA
2013-032-1-200 Van Der Veen	Guidelines for the derivation of values and uncertainties from standard atomic weight intervals	
2013-034-1-500 Gaune-Escard	Mutual Solubility of Rare Earth Metal (Sc, Y, Lanthanides) Bromides in Molten Alkali Bromides	SSED
2013-052-1-024 Kinnan	IUPAC Color Book Data Management	
2013-055-2-024 Straut	Increasing IUPAC's Social Media presence	
2014-012-2-500 Magalhaes	100 Volumes of Plenitude - Celebrating the IUPAC-NIST Solubility Data Series	SSED
2014-027-1-500 Kuselman	Guide for classification, modeling and quantification of human errors in a chemical analytical laboratory	IWPHQA
2012-005-1-500 Hibbert (continued in 2015)	Vocabulary of Concepts and Terms in Analytical Chemistry - the revised Orange Book (4th edition)	OB

## Conferences and Symposia

ISRANALYTICA 2015, 14-15 January 2015 at the David Intercontinental Hotel, Tel-Aviv, Israel.

In conjunction with that major annual event, a Workshop on Human Errors and Quality of Chemical Analytical Results was organised on 13 January 2015 at the adjacent Dan Panorama Hotel by members of the IWPHQA of the Division.

International Workshop on Determining Antioxidants as Reactive Species Scavengers, Istanbul, 27 to 28 October, 2014.

The workshop was organized jointly by the Istanbul University and the Analytical Chemistry Division of IUPAC with Prof. Dr. Reşat APAK (Istanbul University), the workshop chairman.

The 16th International Symposium on Solubility Phenomena and Related Equilibrium Processes was organized by the Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal (KIT-INE), Karlsruhe Germany. This IUPAC-sponsored symposium included a workshop, organised by the SSED, entitled "Solubility and Speciation in Nuclear Waste Disposal".

248th ACS National Meeting, San Francisco, CA – Session: The IUPAC Solubility Data Series: 100 volumes of Solubility Data Online – Wednesday, 13 August, 2014. Members of SSED were responsible for the half day session "The IUPAC Solubility Data Series: 100 volumes of Solubility Data Online" that occurred on the 13th August 2014 in San Francisco, California.