# **Analytical Chemistry Division (V)**

## **Teamwork**

- Issue No. 16 - January 2012

The Analytical Chemistry Division (V) 2010-2011 is happy to present some of its activities since the last issue of Teamwork. *This issue of 'Teamwork' includes:* 

- o 1.- Officers and Division meeting in Glasgow July/August 2009
- o 2.- ACD people 2010-2011
- o 3.-Division Committee Meeting in Aveiro, February 2010
- 4.-The Division and the International Year of Chemistry, IYC 2011
- o 5.- Report to Council 2011
- o 6.-General Assembly in San Juan- Puerto Rico, July/August 2011
- 7.- Interdivisional Working Party for Harmonization of Quality Assurance
- 8.- Subcommittee on Solubility and Equilibrium Data
- o 9.- Subcommittee on pH
- 10.- ACD liaison with other international organisations and groups
- 11 Articles in Chemistry International
- 12- IUPAC Recommendations and Technical Reports 2010—2011
- o 13.- Conferences
- o 14.- Orange Book
- o 15 Stability Constants Database
- o 16.- Projects
- o 17.- ACD people 2012-2013
- 18 Division Committee Meeting in Antwerp, February 2012

#### 1.- Officers and Division meeting in Glasgow July/August 2009

An officers meeting was held during the General Assembly in Glasgow, in the morning of Friday 31st July.

The whole division met in the afternoon of Friday 31st July and on Saturday 1st August. The minutes can be accessed at: <a href="http://old.iupac.org/divisions/V/A1%20-%20Aveiro%20%20ACD">http://old.iupac.org/divisions/V/A1%20-%20Aveiro%20%20ACD</a> %20Glasgow%202009 Minutes.pdf

In addition, a workshop has been arranged on Sunday 2nd August, dedicated to the revision of the Orange Book. It was planned that by the Portugal ACD meeting in Feb 2010 the initial scoping by the "chapter teams" would be completed, i.e. identify people, sub projects, timelines etc. A status update/presentation in February 2010 to take place at ACD meeting

#### 2.- ACD people 2010-2011

President: Fajgelj, Ales

Vice President: Camões, Maria Filomena

Secretary: Hibbert, D. Brynn

**Titular members:**Bunk, David M.; Chai, Zhifang; Maryutina, Tatyana A.; Mester, Zoltán; Motomizu, Shoji; Pingarrón, José M. M.; Sirén, Heli M. M. **Associate** 

members: Balarew, Christo; De Zorzi, Paolo; DeBièvre, Paul; Kim, Hasuck;

Magalhães, Maria Clara; F.Thomassen, Yngvar

National representatives: Aggarwal, Suresh K.; Alam, A. M. Shafiqul; Apak, Resat;

Bode, Peter; Felinger, Attila; Heng, Lee Yook; Jarosz, Maciej; Knochen, Moisés; Labuda, Jan;

Schmidt, Torsten C.

### 3.- Officers and Division meeting in Aveiro, February 2010

Executive Officers' Meeting- 7th February 2010 Division Committee Meeting- 8 and 9 February 2010

The mInutes can be accessed at <a href="http://old.iupac.org/divisions/V/ACD">http://old.iupac.org/divisions/V/ACD</a> %20Aveiro 2010 Minutes.pdf



#### 4.-The Division and the International Year of Chemistry, IYC 2011

Maria Filomena Camões worked with the Committee on Chemical Education in the planning and development of a strategy for a Global Experiment. Regular conference calls and meetings took place and "Water, a chemical Solution" with four activities- Acidity, Salinity, No dirt no germs, Solar still challenge, was launched. Protocols have been prepared and kits have been set up with the support of UNESCO: <a href="http://water.chemistry2011.org">http://water.chemistry2011.org</a>

### 5.- Report to Council 2010-2011

# Aleš Fajgelj, President

#### **Highlights and Executive Summary**

- In the current biennium (2010-2011) a new Subcommittee on pH was established, which
  together with the Division Committee, the Interdivisional Working Party on Harmonization of
  Quality Assurance (<u>WPHQA</u>) and the Subcommittee on Solubility and Equilibrium Data
  (<u>SSED</u>), composes the core bodies of the Analytical Chemistry Division.
- The Division continuous to successfully run a number of divisional and interdivisional projects. Ten projects were completed, 32 are active Divisional projects, and nine are ongoing Interdivisional projects.
- The Division keeps and actively supports its key publication/databases, namely The Compendium of Analytical Nomenclature - Orange Book, the Solubility Database and the Stability Constants Database.
- For the current biennium Division has established focus (interest) groups on Communication, Critical evaluation of data, Electronic resources for IUPAC terminology work, Emerging analytical issues, Metrology, and the Analytical potential of nuclear techniques.
- The Division is actively involved in global harmonization and standardization activities, where metrology in chemistry remains to be the focal topic.
- The Division actively cooperates with number of international organizations and bodies (e.g. BIPM, CITAC, EURACHEM, IAEA, IAM, IUPAP, UNIDO, etc.)

#### 6.- General Assembly in San Juan-Puerto Rico, July/August 2011



Division Presidents (DAC- Ales Fajgelj) receive the IUPAC plaque from IUPAC President Nicole Moreau

## 7.- Interdivisional Working Party for Harmonization of Quality Assurance

Chair (2010-2011): De Zorzi, Paolo

Chair (2012-2013): Fajgelj, Ales

#### 8.- Subcommittee on Solubility and Equilibrium Data

Chair: Magalhães, M. Clara F.

The SSED's Solubility Data Project and the International Symposium on Solubility Phenomena

http://old.iupac.org/divisions/V/502/homepage/index.html

The 14th International Symposium on Solubility Phenomena – Including Related Equilibrium Processes was held from 25 to 30July 2010 in Leoben, Austria, organized by by Prof. Heinz Gamsjäger in conjunction with the 9<sup>th</sup> annual meeting of the SSED.

Traditionally the symposium deals with all aspects of solubility: in and between solids, liquids and gases; new experimental methods for investigation of solubility phenomena, new analytical techniques, new experimental data, prediction of solubilities and phase equilibria by thermodynamic and molecular modelling, correlation to molecular structure, thermodynamic data bases, application of solubility data and phase equilibria in industry, for protection of environment and in geochemistry. The next symposium, 15<sup>th</sup> ISSP will take place in Innsbruck in 2012.

#### 9.- Subcommittee on pH

Taking into account IUPAC leadership in this field, the importance of pH measurements in general, and the historical place of electrochemical methods in the past IUPAC structure, the Analytical Chemistry Division was considered the appropriate organizational entity to host a subcommittee on pH. One immediate task for the subcommittee being to provide thoughtful input into the debate about worldwide experiments for young people in the 2011 International Year of Chemistry.

Chair: Maria Filomena Camões

#### **Terms of Reference**

**A-** The "Subcommittee on pH", SpH, has been founded and will operate in the frame of the IUPAC Analytical Chemistry Division. The initial membership list\* is:

M. Filomena Camões- Pt- fcamoes @fc.ul.pt Paulo Borges- Br- ppborges @inmetro.gov.br Richard Brown- UK- richard.brown @npl.co.uk Paola Fisicaro- F- paola.fisicaro @lne.fr Isabel Fraga- Br- icfraga @inmetro.gov.br M. J. Guiomar Lito- Pt- mjglito @ff.ul.pt Michal Mariassy- Sk- 'mariassy @smu.gov.sk' Martin Milton- UK- martin.milton @npl.co.uk Kenneth Pratt- USA- kenneth.pratt @nist.gov Petra Spitzer- De- Petra.Spitzer @ptb.de

Membership may be revised, seeking representativeness and relevant contribution to the activities.

- **B-** The Division is the home for the designated\* SpH which is responsible for:
  - 1. Fostering an understanding of both the concept of pH and its fundamental importance among the general public.

This includes,

- a) Actively engaging in education and training actions aiming at all age and academic levels,
- b) Production of appropriate educational tools, namely written material that supports.
- 2. Promoting a general understanding of the measurement of pH and the importance of its traceability to the SI among the chemical community as a whole.

This includes,

- a) Participation in public events with the presentation of interesting work results from scientific research and technical development perspectives,
- b) Publication of pertaining data and information in both specialised journals and the media in general.
- 3. Establishing and disseminating the traceability chain for pH measurement by focusing on the primary, secondary and the routine pH measurements relating each one to the respective target uncertainties.

This includes,

- a) Investigation of the factors that limit the uncertainty of the measurement of the acidity function in cells without transference with which the primary measurement per se of pH is realised.
- b) Collecting information on and evaluate models for single-ion activity as candidates to supersede the Bates-Guggenheim convention, the uncertainty of which currently limits the traceability of pH to the SI via the primary measurement method for pH.
- c) Study of the influential parameters for pH meter calibration and pH practical measurement, in cells with diffusion, such as liquid junction potential, indicator and reference electrode (e.g, single and combination electrode assemblies) behavior, reference buffer standards and temperature,
- d) Providing data that enable informed users to assign credible uncertainties in such measurements of the pH of samples encountered in real-world analyses.

4. Addressing new challenges, proposing and undertaking actions that contribute to updating the relevance of pH.

This includes,

- a) Investigation of cost-effective means of disseminating the primary measurement of pH via certified reference materials with compositions nominally identical to the primary standards,
- b) Development and validation of new pH measurement techniques and Equipment,
- c) pH measurement in complex matrices, namely non-aqueous solutions, e.g. in seawater, physiological fluids, bioethanol,
- d) Proposing actions, such as proficiency testing in pH measurement with the use of aqueous and non-aqueous pH reference buffer solutions.

#### 10.- ACD liaison with other international organisations and groups- Biennium 2010-2011

- **a.** Representative to Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)- Prof. D. Brynn Hibbert
- **b.** Committee on Chemical Education (CCE). Prof. M. Filomena Camões (*Task Group Global ExperimentlYC 2011*)
- c. Committee on Chemical Industry (COCI) Dr Zoltán Mester;
- d. Pure and Applied Chemistry Editorial Advisory Board Dr. Ales Fajgelj;
- **e.** International Committee on Weights and Measures/Consultative Committee on the Amount of Substance (BIPM/CCQM) Dr Ales Fajgelj;
- f. ISO-Committee on Reference Materials (ISO/REMCO) Dr Ales Fajgelj;
- g. Joint Committee for Guides in Metrology (BIPM/JCGM) Working Group1 Prof Brynn Hibbert;
- h. Joint Committee for Guides in Metrology (BIPM/JCGM) Working Group 2 Prof Paul de Bièvre;
- i. Inter-Agency Meeting (IAM) Prof Ryszard Lobinski;
- j. Joint Committee on Traceability in Laboratory Medicine (JCTLM) Prof Paul de Bièvre
- **k.** Ad hoc group on redefinition of the mole (Prof Paul de Bièvre)

#### 11.- Articles in Chemistry International

- Analytical Chemistry in Action, Brynn Hibbert, Secretary of Division V, Vol. 32
   No. 4, July-August 2010
- **A century of pH Measurements,** MF Camões, Vol 32, n° 2, March April 2010,

#### 12.- IUPAC Recommendations and Technical Reports 2010-2011

Metallomics: Guidelines for terminology and critical evaluation of analytical chemistry approaches (IUPAC Technical Report)\*
Ryszard Lobinski, J. Sabine Becker, Hiroki Haraguchi, and Bibundhendra Sarkar
Pure Appl. Chem., Vol. 82, No. 2, pp. 493–504, 2010.

doi:10.1351/PAC-REP-09-03-04

The IUPAC-NIST Solubility Data Series: A guide to preparation and use of compilations and evaluations (IUPAC Technical Report)\*,§
Heinz Gamsjäger, John W. Lorimer, Mark Salomon, David G. Shaw, and Reginald P. T. Tomkins
Pure Appl. Chem., Vol. 82, No. 5, pp. 1137–1159, 2010. doi:10.1351/PAC-REP-09-10-33

# IUPAC-IUGS common definition and convention on the use of the year as a derived unit of time (IUPAC Recommendations 2011)\*,\*\*

Norman E. Holden, Mauro L. Bonardi, Paul De Bièvre, Paul R. Renne and Igor M. Villa Pure Appl. Chem., Vol. 83, No. 5, pp. 1159–1162, 2011. doi:10.1351/PAC-REC-09-01-22

# Metrological traceability of measurement results in chemistry: Concepts and implementation (IUPAC Technical Report)\*

Paul De Bièvre, René Dybkaer, Aleš Fajgelj, and D. Brynn Hibbert Pure Appl. Chem., ASAP Article doi:10.1351/PAC-REP-07-09-39

IUPAC/CITAC Guide: Selection and use of proficiency testing schemes for a limited number of participants—chemical analytical laboratories (IUPAC Technical Report)\* llya Kuselman and Aleš Fajgelj Pure Appl. Chem., Vol. 82, No. 5, pp. 1099–1135, 2010. doi:10.1351/PAC-REP-09-08-15

#### Electrochemical nucleic acid-based biosensors: Concepts, terms, and methodology (IUPAC Technical Report)\*

Jan Labuda, Ana Maria Oliveira Brett, Gennady Evtugyn, Miroslav Fojta, Marco Mascini, Mehmet Ozsoz, Ilaria Palchetti, Emil Paleček, and Joseph Wang Pure Appl. Chem., Vol. 82, No. 5, pp. 1161–1187, 2010. doi:10.1351/PAC-REP-09-08-16

Chemical speciation of environmentally significant metals with inorganic ligands.

Part 4: The Cd<sup>2+</sup> + OH<sup>-</sup>, Cl<sup>-</sup>, CO<sub>3</sub><sup>2-</sup>, SO<sub>4</sub><sup>2-</sup>, and PO<sub>4</sub><sup>3-</sup> systems (IUPAC Technical Report)\*

Kipton J. Powell, Paul L. Brown, Robert H. Byrne, Tamas Gajda, Glenn Hefter, Ann-Kathrin Leuz, Staffan Sjöberg, and Hans Wanner

Pure Appl. Chem., Vol. 83, No. 5, pp. 1163–1214, 2011. doi:10.1351/PAC-REP-10-08-09

#### 13.- Conferences

i).- Chemical Education/CCE- Taipei, August 2010 ii).- Euroanalysis 16– Belgrade, September 2011

#### 14.- Orange Book

The third edition, dated 1997, is undergoing revision along the following agreed structure:

Chapter 1-Fundamental concepts and terms(metrology),chemometrics (and statistics),Quality assurance; Chair-Paul DeBièvre,IUPAC liaison- D.Brynn Hibbert (™) Chapter 2-Sampling and sample preparation; Chair and IUPAC liaison - Zoltan Mester (TM) Chapter 3- Methods of analysis depending on measurements of mass and volume Chair and IUPAC liaison- Maria F. Camões(TM)

Chapter 4- Separation Chair- Tatyana Maryutina (AM), IUPAC liaison- Tatyana Maryutina (AM) and Attila Felinger (TM)

Chapter 5- Spectroscopic methods of analysis Chair and IUPAC liaison-Yngvar Thomassen (TM)

Chapter 6- Mass spectrometry Chair and IUPAC liaison- Zoltan Mester (TM)

Chapter 7- Electrochemical methods of Analysis Chair and IUPAC liaison- José M.

Pingarrón, (TM)

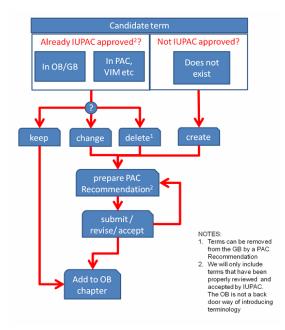
Chapter 8- Radioanalytical Methods; Chair- Zhifang Chai, IUPAC liaison- Peter Bode (AM)

Chapter 9- Surface analysis; Chair- Luisa Maria Abrantes; IUPAC liaison-Maria F. Camões (™)

Chapter 10- Thermal methods of analysis; Chair- Carlos Castro; IUPAC liaison-Maria F.

Camões (™)

Chapter 11- Immuno- and bio-analytical methods of analysis; Chair and IUPAC liaison - Jan Labuda (TM)



## 15.- Stability Constants Database

**Aqueous Solutions**. A package of programs for the quantitative treatment of a wide range of equilibria in solutions of varying backgrounds, ionic strengths and temperatures. <a href="project 2000-003-1-500">project 2000-003-1-500</a>

More information: Academic Software at www.acadsoft.co.uk

#### 16.- Projects

List and status at:

http://www.iupac.org/indexes/Projects/bodies/500

#### 17.- ACD people 2012-2013

A- Elections have taken place for the Division Committee Members for the biennium 2012-2013.

The Nomination Committee consisted of

Chair: Brynn Hibbert

Members: Ryszard Lobinski, Walter Lund, David Moor

The Committee has the following composition:

President: Camões, Maria Filomena

Vice President: Hibbert, D. Brynn

Secretary: Mester, Zoltán Past President: Fajgelj, Ales

Titular members: Balarew, Christo; Felinger, Attila; Labuda, Jan; Magalhães, M. Clara;

Pingarrón, José M. M.; Thomassen, Yngvar

Associate members: Apak, Resat; Bode, Peter; Chen, Yi; Heng, Lee Yook; Kim, Hasuck;

Maryutina, Tatyana A.

**National representatives:** Alam, A. M. Shafiqul; Chande Othman, Othman; Charles, Laurence; Eberlin, Marcos N.; Grudpan, Kate; Hanif, Javed; Mandler, Daniel; Novak, Predrag; Sirén, Heli; M. M.; Torto, Nelson

#### B- Division V nominees for IUPAC Committees 2012-2013:

- a. Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)- Brynn Hibbert:
- b. Committee on Chemical Education (CCE)- Nelson Torto;
- c. Committee on Chemical Industry (COCI)- Zoltán Mester;
- d. Pure and Applied Chemistry Editorial Advisory Board-Ales Fajgelj;

#### C- Division V nominees for the IUPAC representative on external bodies

- e. International Committee on Weights and Measures/Consultative Committee on the Amount of Substance (BIPM/CCQM)- Ales Fajgelj;
- f. ISO-Committee on Reference Materials (ISO/REMCO) -Ales Fajgelj;
- g. Joint Committee for Guides in Metrology (JCGM)- Paul de Bièvre
- h. Joint Committee for Guides in Metrology (JCGM) Working Group 1-Brynn Hibbert;
- i. Joint Committee for Guides in Metrology (JCGM) Working Group 2-Paul de Bièvre;
- j. Inter-Agency Meeting (IAM)- Zoltán Mester;
- k. EUCHEMS- Maria Filomena Camoes + Jan Labuda;
- I. African Network of Analytical Chemists (ANAC)- Nelson Torto m- CITAC Ilya Kuselman

#### D- Division V nominees for IUPAC Committees 2012-2013:

- a. Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)-Brynn Hibbert:
- b. Committee on Chemical Education (CCE)- Nelson Torto;
- c. Committee on Chemical Industry (COCI)- Zoltán Mester;
- d. Pure and Applied Chemistry Editorial Advisory Board- Ales Fajgelj

#### 18 - Division Committee Meeting in Antwerp, February 2012

Executive Officers' Meeting- 5th February 2012
Division Committee Meeting- 6 and 7 February 2012



Minutes will be available soon