



INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Analytical Chemistry Division Report to Bureau – Apr 2017

Prepared by Jan Labuda, Division President

I. Highlights and/or Executive Summary

This should identify items for **discussion and/or decision by the Bureau** and list **Division/Committee priorities for the 2016-2017 biennium and the next one**. It should also cover the major points and **achievements that the Division President/Standing Committee Chair** wishes to convey to the Bureau and Council, since this and part II will most likely be read carefully.

Division priorities and achievements:

- Division Committee permanent activity particularly regarding the transfer of information from the Secretariat and DP to the Div members as well as via mutual contacts of the Div officers, Committee members and reps – 2 letters of the DP, relatively large number of email from DP, but with exceptions rather various activity of some TMs, AMs and NRs.
- Preparation of PAC Recommendations/TRs and the Orange Book revision under the title “Compendium of Terminology in Analytical Chemistry”, Brynn Hibbert, the Editor – at present most of the analytical methods are covered by submitted PAC Recommendations or Technical Reports (see below).
- Progress on individual IUPAC projects following their planned end dates – see list below.
- Participation of the Div reps on the work of other bodies, the Div members/projects chairs on workshops and conferences with information on IUPAC, projects dissemination, and the Div V goals and activities – see list below.
- Division ballot for the next biennium to ensure continuation in the active work.

Item for discussion and/or decision - IUPAC funds for travel in advance:

The Div V officers would like to ask at the Bureau and Council for a possibility to help TMs from developing countries and people who are not able to use an organizational support (e.g. retired people) to attend the GA and Division Committee meeting by covering the travel expenses in advance (as it was in the past). In the case of air tickets even the reimbursement will come long months after the payment.

II. Plans and priorities for the remainder of this biennium, and beyond

Provide some detail regarding your intentions for your Division/Committee and the context within which that work will be done. For example, you might want to describe **the overall strategy of your Division / Committee**, and to include a short section on the activities of **specific bodies** if that seems desirable. You may want to provide **a summary of the number and general types of projects**. You may wish to highlight some **interdisciplinary activities within IUPAC or with outside groups** if these were not covered in part II. You may want to **comment on particular organizational or operational aspects that you think should be brought to the attention of Council**. In short, part III is free-form; you can put into it whatever you wish, preferably without duplication of information from other parts.

The overall strategy is directed to visibility of the Division and SSED as well as quality of the Division products. It concerns:

- a) Finalization of the revision of the Orange Book. - At present, most of the chapters are in a reasonably advanced state when the chapters undergo through the PAC Recommendations/TRs publications. For details see below.
- b) IUPAC projects selection on issues recognized as emerging ones:
 - Finalization of quite long list of running projects, - in 2016 together 32 projects, 6 projects have been completed, 5 projects past the end date, remaining budget was less than 40 % (at present the lowest among the divisions).
 - Selection of new projects within Analytical Chemistry and within the Subcommittee on Solubility and Equilibrium Data (SSED) – at present 3 project proposals under evaluation.
- c) SSED activity and products – for details see below.
- d) Work of the Div V reps in internal and external bodies, particularly:
 - Joint Committee for Guides in Metrology (JCGM) and its Working group 1 and 2.

ACD members on internal and external committees:

Body/ Committee/ Organisation	Membership
<u>Internal</u>	
Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)	Attila Felinger
Committee on Chemical Education (CCE)	Maria Filomena Camoes
Committee on Chemical Industry (COCI)	Jan Labuda
Committee on Publications and Cheminformatics Data Standards (CPCDS)	Brynn Hibbert
Committee on Chemistry Research Funding (CCRF)	Jan Labuda
Pure and Applied Chemistry Editorial Advisory Board (PAC-EAB)	Zoltán Mester
<u>External</u>	
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)	Zoltán Mester
Joint Committee for Guides in Metrology Working Group1 (JCGM WG1)	Steven Ellison, Juris Meija
Joint Committee for Guides in Metrology Working Group 2 (JCGM WG2)	Zoltán Mester, Gunnar Nordin
Inter-Agency Meeting (IAM)	Zoltán Mester
EUCHEMS	Slavica Razic, Jan Labuda
African Analytical Network	Nelson Torto
CITAC	Ilya Kuselman / Aleš Fajgelj
CODATA	Clara M. Magalhães

III. An overall report on Division activities and achievements during 2016-2017 biennium (IUPAC's Mission, Core Values, Goals, activities and Objectives).

This will provide more details in a format that is common to all Divisions and Operational Committees. It will permit interested Bureau members to see the **Division's work in the context of overall IUPAC strategy**. *Note that it is neither necessary nor desirable to include accomplishments under each Goal*, and there is no problem in referring to an activity under more than one Goal where appropriate, but that Bureau and Council should be able to assess the level of alignment with IUPAC's Mission, Core Values, Goals and Objectives.

Keeping the **IUPAC Strategic Plan as "living document"** - this has been discussed in details during the Div V Committee meeting on 19 to 21 March, 2016 in Bratislava, Slovakia.

- *A focus on those aspects of chemistry where global consensus is essential for progress in research, commerce and policy:*

This is performed via:

- a) Longtime and intensive participation of the Div V on all modern aspects of the chemical measurement as stated by the International Vocabulary on Metrology (VIM). This participation covers activities of both Div V directly and external cooperation within JCGM with the WG1 and WG2, and others.
- b) Intensive work the Orange Book re-edition and publication of PAC Recommendations on individual methods of the analytical chemistry.
- c) Div V projects and projects with interdivisional cooperation and participation.

- *Respect for its objectivity and scientific excellence, providing access to the highest levels in the scientific, industrial, and policy communities to represent global chemistry:*

This continues to be performed by Div V representatives at internal and external bodies, interdivisional interaction and collaboration including chemistry education.

- *A worldwide base of volunteers with the best skills and background, recruited by transparent and well-understood processes:*

This continues to be performed by checking the projects task group composition considering skill and geography.

Orange Book re-edition (B. Hibbert):

It represents the main division activity and product during the biennium. A contract with the Royal Society of Chemistry last year, for a submission date of 31 March 2018, expectation 1000 pages (@500 words per page).

Chapter # [3 rd edition #] (present working #)	Title	Editor	State
Chapter 1 [1] (1)	Fundamental concepts and terms (metrology)	Heiner Korte	Draft completed with discussion still ongoing.
Chapter 2 [-] (1a)	Chemometrics and statistics	Brynn Hibbert	Recommendation published. Hibbert, D. B., Vocabulary of concepts and terms in chemometrics (IUPAC Recommendations 2016).

Chapter 3 [-] (2)	Sampling and sample preparation	Janusz Pawliszyn	<p><i>Pure Appl. Chem.</i> 2016, 88 (4), 407-443.</p> <p>TR and Recommendation published</p> <p>Poole, C.; Mester, Z.; Miró, M.; Pedersen-Bjergaard, S.; Pawliszyn, J., Extraction for analytical scale sample preparation (IUPAC Technical Report). <i>Pure Appl. Chem.</i> 2016, 88 (7), 649-687.</p> <p>Poole, C.; Mester, Z.; Miró, M.; Pedersen-Bjergaard, S.; Pawliszyn, J., Glossary of terms used in extraction (IUPAC Recommendations 2016). <i>Pure Appl. Chem.</i> 2016, 88 (5), 517-558.</p>
Chapter 4 [4,6] (3)	Methods of analysis depending on measurements of mass and volume	Maria F. Camões	Nearly completed draft of a TR.
Chapter 5 [9] (4)	Separation	Tatyana Maryutina	Recommendation submitted 28/1/2017
Chapter 6 [10,11] (5)	Spectroscopic methods of analysis	Derek Craston	Suggestion to split into 3 chapters. No drafts as yet.
Chapter 7 [12] (6)	Mass spectrometry	Zoltán Mester	Recently published Recommendation can be used as basis for chapter. Chapter draft in Dropbox.
Chapter 8 [8] (7)	Electrochemical methods of analysis	José M. Pingarrón	<p>Murray, K. K.; Boyd, R. K.; Eberlin, M. N.; Langley, G. J.; Li, L.; Naito, Y., Definitions of terms relating to mass spectrometry (IUPAC Recommendations 2013). <i>Pure Appl. Chem.</i> 2013, 85 (7), 1515-1609.</p> <p>Substantial draft in Dropbox. Being worked on with view to early submission.</p>
Chapter 9 [16] (8)	Radioanalytical methods	Peter Bode	Attempts to synthesize Chai and Bonardi texts. Some recent activity but main task yet to get underway.
Chapter 10 [17] (9)	Surface Analysis	Takae Takeuchi	Draft in preparation by new team. List of terms but which need completion.
Chapter 11 [5] (10)	Thermal methods of analysis	Carlos Castro	?
Chapter 12 (11)	Bioanalytical methods	Jan Labuda	Revision to Recommendation submitted 21/2/2017.
Chapter 13 [18]	Quality Assurance	Ulf Örnemark	Substantial draft in Dropbox. Close working with Chapter 1 team.

SSED subcommittee activity report (D. Shaw):

The **17th International Symposium on Solubility Phenomena and Related Equilibrium Processes** occurred in the University of Geneva, Geneva, Switzerland from the 25th to the 29th July 2016. The conference was attended by around 110 people, and had 13 plenary lectures, 40 oral communications and 38 posters. Three IUPAC prizes for the best poster communications were given.

The 2016 Franzosini Award was given to David Fellhauer in recognition of his contribution to the IUPAC Solubility Data Project. He was honored at the 15th Annual Meeting of the IUPAC Subcommittee on Solubility and Equilibrium Data held in Geneva, Switzerland on the 24 July 2016 and which took place during the 17th International Symposium on Solubility Phenomena and Related Equilibrium Processes.

The 42nd Annual meeting of the former Solubility Committee and 15th of the SSED was held in conjunction with the 17th ISSP on the 24th July 2016 in Geneva, Switzerland. This meeting was attended by 22 members of SSED.

Subcommittee on pH - SpH report (M. F. Camoes):

In the frame of the activities and plans of SpH: Traceability of pH Measurements for Application in Fundamental and Applied Science, the milestones of ongoing Project N° 2013-013-1-500- pH Measurement in Seawater (M F Camões chair) were presented, starting from IUPAC Recommendations 2002: Measurement of pH. Definition, Standards, and Procedures. An account of publications, further research, and collaboration with relevant stakeholders is given. In 2016, the contribution “Metrological challenges for measurements of key climatological observables. Part 3: Seawater pH” has been published as the product to Global climate changes.

Report of the JCGM-WG1 (Juris Meija (NRC), Stephen Ellison (LGC)):

The Joint Committee for Guides in Metrology (JCGM) is tasked with maintaining and promoting the use of the “Guide to the Expression of Uncertainty in Measurement” (known as the GUM) and the “International Vocabulary of Metrology” (known as the VIM). The JCGM operates through two working groups: JCGM-WG1, with responsibility for the GUM, and JCGM-WG2, with responsibility for the VIM. JCGM has eight member organizations which include IUPAC. IUPAC is currently represented in the JCGM-WG1 by Stephen Ellison (LGC, UK) and Juris Meija (NRC, Canada).

The June 2016 meeting of WG1 focused primarily on two items of business; actions following member and NMI comment on the 2015 Committee Draft of a revision of the GUM, and steps towards a further JCGM Supplement covering the construction of a ‘measurement model’ suitable for evaluation of measurement uncertainty. The working group acknowledges that the proposed GUM2 has failed to adequately communicate the rationale for revision of the GUM.

Actualization of the Division Web page:

Division Vicepresident Zoltan Mester is currently working on a new Web page of the Division V.

SSED Web Page (David Shaw, February 2016):

Over the last several months the SSED web page has been brought up to date and reorganized to better reflect the full range of the subcommittee’s activities. Concise sections of the page now present our work in the following areas:

- Solubility Data Series with a full, current list of published volumes,
- Stability Constant Database,
- International Symposia on Solubility Phenomena with a list of all past symposia,
- The Franzosinni Award with a complete list of recipients.

A schedule of future meetings is now current and minutes of all meetings from 2001 through 2016 are posted. We are currently working to revise our list of participants and ensure that all contact information is current. We are also considering other activities which might be added to the page.

IV. **Tabular material**

This should include a list of publications. It might also include a list or summary of conferences and symposia organized by the Division or its component bodies. It should include a list of all current Division projects. Again, this part is open-ended.

List of publications:

Hibbert, D. B., Vocabulary of concepts and terms in chemometrics (IUPAC Recommendations 2016). Pure Appl. Chem. 2016, 88 (4), 407-443.

Poole, C.; Mester, Z.; Miró, M.; Pedersen-Bjergaard, S.; Pawliszyn, J., Glossary of terms used in extraction (IUPAC Recommendations 2016). Pure Appl. Chem. 2016, 88 (5), 517-558.

Poole, C.; Mester, Z.; Miró, M.; Pedersen-Bjergaard, S.; Pawliszyn, J., Extraction for analytical scale sample preparation (IUPAC Technical Report). Pure Appl. Chem. 2016, 88 (7), 649-687.

Labuda, J.; Bowater, R.P.; Fojta, M.; Gauglitz, G.; et al., Terminology of bioanalytical methods (IUPAC Recommendations 201x). Pure Appl. Chem. Revision to Recommendations submitted 21/2/2017.

Dickson, AG.; Camoes, MF.; Spitzer, P.; Fisticaro, P.; Stoica, D.; Pawlowicz, R.; Feistel, R., Metrological challenges for measurements of key climatological observables. Part 3: Seawater pH. Metrologia 2016, 53, R26-R39.

Oracz, P., Góral M., Wiśniewska-Gocłowska B., Shaw DG., Maczyński A., IUPAC-NIST Solubility Data Series. 101. Alcohol + Hydrocarbons + Water. Part 2. C₁-C₃ Alcohols + Aliphatic Hydrocarbons, J. Phys. Chem. Ref. Data 2016, 45, 033102

Oracz, P., Góral M., Wiśniewska-Gocłowska B., Shaw DG., Maczyński A., IUPAC-NIST Solubility Data Series. 101. Alcohol + Hydrocarbons + Water. Part 3. C₁-C₃ Alcohols + Aromatic Hydrocarbons, J. Phys. Chem. Ref. Data 2016, 45, 033103

Critical Evaluation of Equilibrium Constants of 4f Metal Mixed Complexes with Acidic (Chelating) Ligands in Combination with Various Organophosphorus O-donor Molecules Chem. Internatl. 2016, 38, 24.

Kuselman, I.; Pennechi, F. Human Errors in a Routine Analytical Laboratory—Classification, Modeling and Quantification: Overview of the IUPAC/CITAC Guide, Chem. Internatl. 2016, 38, 27.

International Vocabulary of Metrology, Chem. Internatl. 2016, 38, 25.

Summary of conferences and symposia:

Workshop “Advances in Analytical Chemistry” (Jan Labuda chair) was held on 21 March, 2016, in Bratislava, Slovakia, just after the Division V Committee meeting. The scope of the workshop was to provide state-of-the-art of specific topics of modern Analytical Chemistry, its concepts and associated terms together with identification of its future tasks. The lectures by nine Div V Committee members have presented the situation in current development of both Analytical Chemistry as the science and analytical methods, an experiences of scientists and researchers in different areas of analytical chemical measurement at universities and research laboratories, and also a way for further education particularly university teachers, research staff and young chemists in Slovakia and the Mid-Europe region.

9th International Symposium on New Trends in Chemistry: Analytical Chemistry for Better Life was held on January 02-05, 2017 at the Cairo University, Cairo, Egypt (Chair: Dr. Mothaza Khater, Support: Egyptian Society of Analytical Chemistry Egyptian Society). Division V was represented by Érico M. M. Flores - Associate Member (Brazil) and Medhat Al-Ghobashy - National Representative (Egypt). Many scientists have attended this conference, including the editors or editorial board members of *Analyst* (RSC), *J. Anal. At. Spectrom.* (RSC), *Arabian J. Chem.* (Elsevier) and *TrAC* (Elsevier).

The 3-rd biannual international IUPAC/CITAC Workshop on Quality and Metrology of Chemical Analytical Results (planned as a milestone of IUPAC project 2016-007-1-500, Ilya Kuselman chair), was organized with participation of the Israel Analytical Chemistry Society (IACS) and the Israel Laboratory Accreditation Authority (ISRAC) on 23 January 2017 in Kfar Maccabiah, Israel. The event was sponsored by Sigma-Aldrich Corporation (a part of Merck today) and arranged by Bioforum Ltd.

The discussion included the following topics:

- use of results of human error study at validation of an analytical method;
- evaluation of measurement uncertainty of the test (analytical) results as a part of the method validation task;
- evaluation of probabilities of false decisions at conformity assessment of test results obtained by the method under validation.

The round-table discussion was held “How can validation be planned to provide a method user with maximum information?” More details about the workshop and presentations are available from <http://bioforumconf.com/satellite-event2017/workshop-program2017>.

4th FUE International Conference on Pharmaceutical Sciences – January 30 – February 02, 2017, Future University in Egypt, Cairo, Egypt (Chair: Dr. Seham ElKhesheh, Support: FUE and IUPAC). Division V was represented by Érico M. M. Flores - Associate Member (Brazil) and Medhat Al-Ghobashy - National Representative (Egypt). It was a big conference with the attendance of scientists of many countries, including representatives of pharmacopoeias, health authorities and industrial pharmaceutical suppliers.

Proposed-tentative meeting for IUPAC Advertising in Brazil after the IUPAC 2017 GA in São Paulo at Federal University of Santa Maria, UFSM, Brazil. Organizer: Érico M. M. Flores - Div. V Associate Member (Brazil). The goal is to join some of the division meeting and GA participants during a one-day meeting in Santa Maria, RS to disclose IUPAC activities for young researchers in Santa Maria.

List of all current division projects:

Project Numbers	Planned End Date
2001-063-1-500 Smith	30-Jun-2017
2002-044-1-500 Scharlin	31-Dec-2017
2005-035-2-500 Belli	31-Dec-2017
2008-025-1-500 Filella	31-Dec-2017
2009-006-1-500 Ellison	31-Dec-2017
2010-030-1-500 Chai	30-Jun-2013
2010-052-1-500 Pingarron	31-Dec-2017
2011-031-1-500 Voigt	30-Jun-2017
2011-046-1-500 Maryutina	31-Dec-2017
2011-047-1-500 Labuda	31-Dec-2017
2011-065-3-500 Bendova	1-Aug-2014
2012-004-1-500 Gamsjager	31-Dec-2017
2012-008-1-500 Hefter	31-Dec-2017
2012-022-1-500 Eysseltova	1-Sep-2017
2012-030-1-500 Guminski	1-Sep-2017
2012-031-1-500 Shaw	31-Dec-2016
2013-013-1-500 Camoes	1-May-2016
2013-025-2-500 Westwood	31-Dec-2017
2013-034-1-500 Gaune-Escard	31-Dec-2017
2014-025-1-500 Hibbert	31-Mar-2017
2015-008-2-500 Apak	31-Dec-2017
2015-020-2-500 Leito	30-Jun-2018
2015-021-1-500 Hibbert	30-Jun-2017
2015-024-2-500 Hibbert	31-Dec-2017
2015-028-2-500 Camoes	30-Sep-2016
2015-044-2-500 Bendova	31-Dec-2018
2015-051-1-500 Voigt	30-Jun-2018
2016-003-1-500 Atanassova	30-Jun-2018
2016-004-1-500 Filella	30-Jun-2017
2016-005-1-500 Nordstrom	30-Jun-2018
2016-007-1-500 Kuselman	30-Jun-2018
2016-043-1-500 Shaw	31-Dec-2017

New projects proposals submitted for evaluation:

2016-041-1 Filella (SSED)

2016-042-1 Filella (SSED)

2017-005-1 Labuda