



International Union of Pure and Applied Chemistry
Analytical Chemistry Division

Division Committee Meetings
at the 47th IUPAC General Assembly
Harbiye Military Museum.
Istanbul, Turkey
Friday, 9th - Saturday, 10th August (AM & PM)

Minutes

Present

Prof. Maria F. Camões	TM - President	
Prof. D. Brynn Hibbert	TM - Vice President	
Dr. Zoltán Mester	TM - Secretary	
Dr. A les Fajgelj	TM - Past President	
Prof. Christo Balarew	TM	
Prof. Yngvar Thomassen	TM	
Prof. Attila Felinger	TM	Felinger@ttk.pte.hu
Prof. M. Clara F. Magalhães	TM	mclara@ua.pt
Jan Labuda	TM	jan.labuda@stuba.sk
Paul De Bièvre		paul.de.bievre@skynet.be
Nelson Torto	NR	n.torto@ru.ac.za
Yi Chen	AM	chenyi@iccas.ac.cn
Resat Apak	AM	rapak@instabul.edu.tr
Godfred Darko	YO	Gdarko.sci@knust.edu.gh
Take Takeuchi	YO	Takeuchi_t@cc.nara-wu.ac.jp
Richard Tia	YO	richtiagh@yahoo.com
Lee Wah Lim	YO	lim@gifu-u.ac.jp
Christine Straut	YO	cmstrau@sandia.gov

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Mark Kinnan		mkinna@sandia.gov
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Apologies

Prof. José M. Pingarrón	TM
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Visits:

Friday 9th August 2013

10 to 4pm Colin Humphry from RSC,

4 pm Mark Cesa IUPAC Bureau

4.20pm Paul De Bièvre from Belgium delegation and as JCGM representative

Saturday 10th August

9am Juris Meija from ICTNS

also Mai-Huang Chiu chemistry education (CCE)

Welcome and arrangements

Introduction of participants

1. Approval of Agenda

Agenda approved

2. President remarks

The President welcomed so many Young Observers and invited them to take a full part in the discussions of the Division.

3. Reports from:

- a. Division Meeting, 5th -7th February 2012, Elzenveld Conference Venue, Antwerp, Belgium.

Minutes reviewed by MFC and approved

- b. Bureau Meeting, 13th -15th April 2012, University of Leiden, Netherlands.

MFC presents key points:

Discussion on revision of the SI. Support for a general IUPAC project with Div I , II, V ICTNS, particularly on the mole.

- c. Bureau Meeting, 18th – 21st April 2013, GDCh, Frankfurt, Germany

MFC: Note that project publication should be in PAC unless good reason.

AF: Div V publishes regularly in PAC with high impact. Notes that PAC has open access for Recommendations and Technical Reports. Conference papers are pay per view.

BH: Emphasised that any published report on a funded project must be in PAC. Div V key activity is the production of solubility data. What are the publication arrangements for that?

MCM: Solubility has been published by NIST in the last 15 years. It is a joint IUPAC – NIST project, so has a special dispensation to publish separately. Volume 99. Not really a paper. It is more like a database.

4. Report from Subcommittees

a, Report from Subcommittee on Solubility and Equilibrium Data (SSED)- Maria Clara Magalhães

MCM's report attached

SSED 40 year history

Solubility and equilibrium two committees joined
4 papers/mention of CI (of ISSP conference in China)
4 more mention of Lawrence Clever *in memoriam*.

Main activity IUPAC NIST solubility data series. Volumes 93-99 published. Looking forward to the 100th volume.

In the biennium the subcommittee has completed 9 projects, few more to be completed till the end of the year.

ZM : Can we get the access to usage statistics from NIST?

Action on *MCM*: Obtain information on solubility data access statistics for next report.

b. Report from WPHQA by AF

AF presented a brief historical overview of the WP. Discussed the involvement and interplay between IUPAC, ISO and AOAC.

Recommendations drafted by the WP are the key product. Proficiency testing document collected over 170 citations!

Report from WP meeting on August 8, 2013

A change of title of the WP to reflect emerging concerns and *modus operandum* of the WP was suggested. The proposed new name is Interdivisional Working Party on Quality Assurance and Metrology. First some justifications for its continued existence were discussed.

Justifications for Existence

1. Requirements for Quality Assurance in the field are increasing
2. Implementation of Guides for Metrology (VIM and GUM) in IUPAC (not done at present)

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3. Building bridges on the matters concerned between IUPAC and other communities in chemistry (CITAC, EURACHEM, ISO-REMCO, CCQM, ...)

Potential Members:

1. Ales Fajgelj, Ilya Kuselman, René Dybkaer, Paul De Bièvre, Heiner Korte
2. Ex-officio members: Brynn Hibbert

Current projects:

1. Process mapping of gamma ray spectrometry (finished to be PAC formatted)
2. Human Errors (with CITAC)
3. Guidance for single laboratory validation (Ellison)

Projects envisaged:

1. Organize and maintain website.
2. Organizing Workshops in Bern (CH) Autumn 2014 or Spring 2015)
3. Working out Metrological Traceability Chains for Measurement Results in Chemistry (in cooperation with other Divisions)
4. Contribute to revision of Orange Book

Facilitate implementation of VIM and GUM within IUPAC

ZM : Should Metrology or Measurement Science be in the name

YT: Offer an example of human errors of misuse of information.

Motion to support change the name of WP to Interdivisional Working Party on Quality Assurance and Metrology.

Motion carried.

c. Report from pH working group by *MFC*

It is a relatively new group compared to Solubility or the WP.

The major activity of the team has been project definition. A project on pH measurement in sea water was launched in February 2013.

5. Reports from Task Groups (OB)- *BH*

BH

Flagship products of IUPAC are the color books. Orange book is the product of Analytical Division, which was last updated in 1997, with a PDF version created in 2002.

OB revision

New OB will be collection of defined concepts with terms associated with analytical chemistry. It will contain 11 (possibly 12) new chapters and it will be method based.

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YT: Propose that Chapter 5 be split into separate atomic and molecular spectroscopy chapters. BH remarked this was up to the leader of the chapter (YT). The individual chapters are run through the project system.

Discussion on title of the new edition of the OB.

Approval chain discussed. It was confirmed that the preferred route to for individual chapters is still a PAC publication before lifting new/updated terms into OB.

PDB

It would be ideal if terminology experts could be involved in the projects.

ZM

We are bringing in speaker from ICTNS (Juris Meyer) for terminology guidance.

MFC

Louisa Maria Abrantes, leader of Chapter 9 (surface analysis) has tragically passed away. Her efforts were recognized by a moment of quiet reflection.

MFC said there was a problem accessing her files, and we need a new lead. (Note from BH, Prof Jim McQuillan has agreed to take on this task with a draft to be delivered by end 2014)

Chapter 10. slow progress, no update

Chapter 7 first draft prepared with some progress

Chapter 3 no progress since last report in Belgium

BH: Chapter 4 Little information

Action on OB projects: by December 31, 2013 submit to BH complete list of terms

6. Review of actions arising from the ACD meeting in Antwerp, 2012- Zoltán Mester

ZM reviewed all action items. All were carried out / met.

7. Review of Project Progress Reports

a. Division projects - Brynn Hibbert

Project	Task Chair	Spent	Budget	Over/ (Under) Budget	% of Budget	Planned End Date	e-mail	Report received /Comments
2001-063-1-500	Smith	365	5,000	(4,635)	7%	31-Dec-2010	r.m.smith@lboro.ac.uk	2012-12-19 Fold into OB Chromatography chapter 2011-046-1-500
2002-002-2-500	Labuda	5,000	5,000	-	100%	31-Dec-2011	jan.labuda@stuba.sk	Finished PAC tech report 16 December 2012
2003-015-2-500	Bonardi	8,447	21,000	(12,553)	40%	31-Dec-2010	mauro.bonardi@mi.infn.it	TERMINATE
2003-056-2-	Murray	6,700	7,100	(400)	94%	30-Sep-2012	kkmurray@lsu.edu	manuscript accepted by PAC 2013-03-31

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500								
2005-035-2-500	Belli	2,617	6,000	(3,383)	44%	31-Dec-2012	maria.belli@apat.it	TERMINATE
2007-010-2-500	Bode	-	6,500	(6,500)	-	31-Dec-2011	p.bode@tudelft.nl	TERMINATE
2008-002-1-500	Hibbert	4,695	5,000	(305)	94%	30-Jun-2012	b.hibbert@unsw.edu.au	2012-12-20 Request roll into OB Chapter 1 2012-007-1-500
2008-031-1-500	Apak	5,500	5,500	-	100%	31-Dec-2010	rapak@istanbul.edu.tr	2012-12-18 PAC report submitted 2012-08-01 Published
2009-006-1-500	Ellison	-	4,800	(4,800)	-	31-Dec-2011	s.ellison@lgc.co.uk	email sent 2013-04-02, Aug 10 2013 email from Ellison PROLONG 2015-12-31
2009-010-3-500	De Zorzi	-	6,000	(6,000)	-	31-Dec-2012	paolo.dezorzi@isprambiente.it	email sent 2013-04-02 TERMINATE
2010-030-1-500	Chai	4,007	4,000	7	100%	30-Jun-2013	chaizf@ihep.ac.cn	2012-12-17 draft submitted
2010-052-1-500	Pingarro n	600	2,000	(1,400)	30%	31-Dec-2013	pingarro@quim.ucm.es	email sent 2013-04-02 PROLONG 2015-12-31
2010-061-2-500	Malek	6,988	7,000	(12)	100%	1-Jun-2013	memalek@yahoo.com	email sent 2013-04-02
2011-046-1-500	Maryutin a	-	5,100	(5,100)	-	31-Dec-2013	marvutinata@vrd.ru	email sent 2013-04-02 PROLONG 2015-12-31
2011-047-1-500	Labuda	-	5,100	(5,100)	-	31-Dec-2013	jan.labuda@stuba.sk	2013-01-02 PROLONG 2015-12-31
2011-063-1-500	Pawliszyn	-	5,000	(5,000)	-	31-Dec-2015	janusz@uwaterloo.ca	2013-01-04 PROLONG 2015-12-31
2012-007-1-500	DeBievre	1,461	3,500	(2,039)	42%	1-Mar-2015	paul.de.bievre@skynet.be	2012-12-19

Comment [PDB1]: De Bièvre

b. SSED projects-Maria Clara Magalhães

2002-009-2-500 Gauglitz terminate
 2002-044-1-500 Scharlin Extended 2015 [Alex wise](#) [de Vischer](#)
 2006-034-1-500 Clever [and Battino](#) Extended 2015
 2007-045-1-500 Fogg extended [ed](#)
 2007-047-1-500 Sazonov terminate
 2008-025-1-500 Filella extended [ed](#)
 2010-050-1-500 Goral extended [ed](#)
 2011-031-1-500 Voigt extend

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2011-043-1-500 [chair changed](#) Goral to [David Shaw](#) extended
2012-006-1-500 Lorimer extend
2012-025-1-500 Acree [Extend](#)
2011-06547-31-500 [Bendová-Labuda](#) extend

- c. WPHQA projects -*Ales Fajgelj*
- d. Interdivisional projects, Projects under completion - *BH*

PDB asked for \$2,000 for project extension. Will be considered at the end of biennium.

YT : why is solubility is in Anal Chem and not in physical chemistry division ?

Mark Cesa; SSED could be funded from Div I budget.

AF: SSED represents very good value to the division and IUPAC in general.

Christine Straut: How does IUPAC relate to other standard setting organizations?

BH: IUPAC is one of the standard setting organizations. For example it sits with ISO, IUPAP, ILAC, BIPM, IFCC, and IEC on the JCGM.

- e. Projects with difficulties or with limited progress- *Brynn Hibbert*

Listed and discussed.

- 8. Short reports from liaisons throughout the biennium
 - a. Interdivisional Working Party on Harmonization of Quality Assurance (WPHQA)- *Ales Fajgelj*

AF: Discussed the interaction with other technical committees including CITAC (human error project), ISO REMCO and CCQM.

- b. Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) - *B. Hibbert*;

BH: Issues around the effective representation. Mid-biennium meetings are a problem for unfunded Division reps to participate.

PDB: VIM, new 2012 edition. Annotated VIM coming out (likely 2014)

- c. Committee on Chemical Education (CCE) - *Nelson Torto*

NT: Issue of attendance as no divisional support to attend meetings. No good communications with CCE.

MFC- reiterated the importance of divisional participation in CCE

Christine Straut: use modern communication tools (tele/video-conferencing)?

- d. Committee on Chemical Industry (COCI) - *Zoltán Mester*
No report

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- e. Pure and Applied Chemistry Editorial Advisory Board- *Ales Fajgelj*
Brief report. Issues around new publishing arrangements were discussed earlier.
 - f. International Committee on Weights and Measures/Consultative Committee on the Amount of Substance (BIMP/CCQM) - *Ales Fajgelj*
Report on the April 2013 CCQM meeting in Sevres.
 - g. Joint Committee for Guides in Metrology (BIPM/JCGM) - *Brynn Hibbert*
BH: Current discussion about 'VIN', which will deal with qualitative examination of nominal properties.

JCGM : WG1 (GUM) IUPAC bringing practical problems to WG1
WG2 VIM Both documents will be revised.
Discussion on atomic weight commission request to give guidance on uncertainty of atomic weights.
 - h. Inter-Agency Meeting (IAM) –*Zoltan Mester*
ZM reported on the March 2013 Budapest meeting.
Meeting minutes will be posted on Dropbox.
 - i. Joint Committee on Traceability in Laboratory Medicine (JCTLM)-
No IUPAC representative
-

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9. New project proposals- *M Filomena Camões*

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Project #	Task group chair	Submitted	Budget requested	Comments	awarded
2013-034-1 Mutual Solubility of Rare Earth Metal (Sc, Y, Lanthanides) Bromides in Molten Alkali Bromides	M Gaune-Escard	11/07/2013	\$5,000	SSED Also sent Div 2	4000
2013-032-1 Guidelines for the derivation of values and uncertainties from standard atomic weight intervals	A van der Veen	01/07/2013	\$5,000	Also sent to Div 1, 2	3000
2013-025-1 Methods for the SI Value Assignment of the Purity of Organic Compounds for use as Primary Reference Materials and Calibrators	S Westwood	30/05/2013	\$11,000	2 reviews received 2013-07-11	2000
2013-024-1 Unequivocal Identification of Compounds with Biological Activity of Significance in Food Chemistry	R Molyneux	14/06/2013	\$5,000	Also sent Chemistry and the Environment Division (6)	
2013-015-1 Methods to evaluate the scavenging activity of antioxidants toward reactive oxygen and nitrogen species (ROS/RNS)	R Apak	27/03/2013	\$5,000	Also sent Div 7. According to July list this is awaiting Division recommendation	5000
2012-030-1 Rare Earth Metal (Sc, Y, Lanthanoids) Fluorides in Water and Aqueous Systems - IUPAC NIST Solubility Data Series	C Guminski	03/07/2012	\$2,000	SSED Awaiting Division assessment	\$2,000
2012-022-1 Solubility in Systems with Lithium and/or Sodium Nitrates Part 2 - Sodium Nitrates	J Eysseltova	25/04/2012	\$2,000	SSED Awaiting Division assessment	\$2,000
paul			2000		2000
			\$37,000		\$20,000

PDB : Raised issues around the redefinition of mole. See [Dropbox](#)

AF: what is the role for ACD in this debate?

JL: Noted Eurochem document on the redefinition of the mole. See [Dropbox](#)

AF: How and who should be involved in the up and coming project on redefinition?

MFC: ACD has been always on the record requesting interdivisional project on this. This should not be a political but a highly technical problem

AF: ACD has been following this issue for many years

BH: Presented the ACD position on redefinition (document created in 2012 in Antwerp)

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10. Division membership and structure for 2014 – 2015 biennium

11. Name	Proposed Status	Proposed Term	NAO
Prof. D. Brynn Hibbert	TM - President	2014-2015	Australia
Prof. Jan Labuda	TM - Vice President	2014-2015	Slovakia
Dr. Zoltán Mester	TM - Secretary	2012-2015	Canada
Prof. Maria F. Camões	TM - Past President	2014-2015	Portugal
Prof. Christo Balarew	TM	2012-2015	Bulgaria
Prof. Yi Chen	TM	2014-2015	China
Prof. Attila Felinger	TM	2012-2015	Hungary
Prof. Hasuck Kim	TM	2014-2015	Korea
Prof. Clara Magalhães	TM	2014-2015	Portugal
Prof. Heli M. M. Sirén	TM	2014-2015	Finland
Prof. Resat Apak	AM	2014-2015	Turkey
Prof. Peter Bode	AM	2014-2015	Netherlands
Prof. Yook Heng Lee	AM	2014-2015	Malaysia
Dr. Tatyana Maryutina	AM	2014-2015	Russia
Dr. Nelson Torto	AM	2014-2015	South Africa
Dr. Ales Fajgel	AM	2014-2015	Slovienska
Prof. A. M. Shafiqul Alam*	NR	2014-2015	Bangladesh
Prof. Marcos N. Eberlin	NR	2014-2015	Brazil
Prof. Predrag Novak	NR	2014-2015	Croatia
Prof. Laurence Charles	NR	2014-2015	France
Prof. Daniel Mandler	NR	2014-2015	Israel
Dr. Javed Hanif	NR	2014-2015	Pakistan
Paul De Bievre	NR	2014-2015	Belgium
Prof. Othman Chande Othman	NR	2014-2015	Tanzania
Prof. Kate Grudpan	NR	2014-2015	Thailand
Prof. David G. Shaw	NR	2014-2015	United States
	10 TMs, 6 AMs, 10 NRs		

AM = Associate Member
 NR = National Representative
 TM = Titular Member

AF create observer category !!

Try to added to IUPAC membership list

12. ACD representatives to other IUPAC bodies, external committees 2014 – 2015

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AF Acknowledgement from corporate IUPAC need

- a. Representative to Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) Brynn Hibbert;
- b. Committee on Chemical Education (CCE) Yi Chen;
- c. Committee on Chemical Industry (COCI) Christo Balarew;
- d. Pure and Applied Chemistry Editorial Advisory Board Nelson Torto;
- e. International Committee on Weights and Measures/Consultative Committee on the Amount of Substance (CIPM/CCQM) Aleš Fajgelj;
- f. ISO-Committee on Reference Materials (ISO/REMCO) Aleš Fajgelj;
- g. Joint Committee for Guides in Metrology (JCGM) Paul De Bièvre
- h. Joint Committee for Guides in Metrology (JCGM WG1) Working Group1 Brynn Hibbert;
- i. Joint Committee for Guides in Metrology (JCGM WG2) Working Group 2 Paul De Bièvre;
- j. Inter-Agency Meeting (IAM) Zoltán Mester;
- k. EUCHEMS – Filomena Camões + Jan Labuda
- l. African analytical network – Nelson Torto
- m. CITAC, Ilya Kuselman/ Aleš Fajgelj

YELLOW for approval from Bureau

President: Clarification on IUPAC reps to external organizations discuss with Director!

13. Review of Division operations –M Filomena Camões

- a. Division funds
Under new project proposal (all funds exhausted for the biennium)
About \$60K/2y , 70% /30% project/ops
- b. Division priorities and core business
OB, WP refocus
- c. Task Groups
Create “observer category”

14. Division key products - All

- a. SC-database
Meeting on databases (Aug 10 , 2013), maintenance, hosting etc
- b. Orange Book (*separate meetings have been organized on this topic*).
- c. Division brochure
- d. CI articles
- e. Web page
Single person contact: ZM all web related issues from DivV
- f. Teamwork
17th edition
http://www.iupac.org/fileadmin/user_upload/divisions/V/Teamwork/Teamwork_July_2013.pdf

- g. Conferences and workshops
No sponsorship request
- h. Any other initiative

15. Next ACD meetings

AFel: March 2013, end of the month, hosted by the Hungarian Academy of Sciences, Pécs, Hungary

16. AOB

Visits from other IUPAC bodies:

a, Mai-Huang Chiu chemistry education (CCE).

Introduced the CCE.

Projects: standards for secondary schools in chemistry educations

-Chemistry ambassadors

-Flying chemists

MFC :Supported the involvement of Division members with CCE

YT : Any project educating the text book writers?

PBD: The CCE should consider dealing with teaching the new approach to atomic weight ranges

PDB: Redefinition of mol and kg. There are many problems of teachability with the proposed redefinition of the SI.

BH: Joint committee on guides to metrology working group 1 (JCGM-WG1) delivered opinion on uncertainties associated with atomic weight ranges to CIAAW.

b, COCI Collin Humphry

Applied chemistry group

Capacity building (training for safety in developing world).A workshop for young people who participated is organised.

Chemistry image.

Noted Tuesday World Chemistry Leadership Meeting for young people. Discussed role of IUPAC in the future, or for that matter the role of chemistry in the future.

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c, ICTNS Juris Meija

Gave presentation on “Terminology – general principles”

BH : Should IUPAC adopt the ISO over the present Oxford style for definition? He will prepare a position paper on this with examples.

AF: The IUPAC metrological traceability paper has followed these rules but often commented that is too complicated.

BH : Some example definitions will be provided and critiqued at next OB meeting

Action on *BH*: contact chapter leads and ask them to submit 5 definitions by end of January 2014.

MFC: Portuguese science wiki, scientific correctness and clean language.

JM : Offered to look at first few definitions for consistency with suggested approach.