

IUPAC DIVISION VII
Chemistry and Human Health

Draft Minutes Division VII Meeting 2017
San Paulo, Brazil
IUPAC 49th General Assembly

Location:

WTC Events Center
Av. Nações Unidas, 12551 - Cidade Monções
San Paulo- Brazil

Date

Saturday, July 8, 2017 (9:00-17:30h)
Sunday, July 9, 2016 (8.00-18:30h)

Attendees

Tom Perun (President) (TP), Vincenzo Abbate (VA), Nestor Carballeira (NC), Rita Cornelis (RC), A. Ganesan (AG), Vladimir Gubala (VG), Helle Møller Johannessen (HMJ), Linda Johnston (LJ), Geok Bee Teh (Sharon, GBT).

Guests: Brandon Presley (BP), Doug Templeton (DT) only on Sunday July 9.

Observer: Ester Sztein (ES) intermittently.

Occasional Skype participant: Mike Schwenk (MS).

Short visits from the IUPAC Past President Marc Cesa, the IUPAC Secretary General Richard Hartshorn and the Treasurer Colin Humphris

Apologies

Mike Schwenk (secretary) (MS), Edmond Differding (ED), John Duffus (JD), Janos Fisher (JF), Chulbom Lee (CL)

1. Welcome and Introductions

T. Perun, Division President, welcomes the attendees. Each of them introduces him/herself.

2. Approval of Agenda

The agenda is approved

3. Approval of Minutes of Previous Meeting (Copenhagen 2016)

The minutes of the Division meeting in Copenhagen were accepted in tacit agreement

4. Report of the Division President

TP outlined and updated the activities of the Division in a poster and slides. The poster was then exhibited during a poster session of the 46th IUPAC World Chemistry Congress held in Sao Paulo, 9 - 14 July 2017.

TP noted that IUPAC needs to attract more industry-based members and to seek more collaboration with industry. Great acknowledgement was expressed for JF for his successful industrial engagement, and leadership of the Drug Discovery and Development subcommittee. His medicinal chemistry books receive high, worldwide recognition. ES suggested that we should interview JF and figure out what makes his approach so successful. JF may point out the selling points that we could use in engaging with other companies.

BP mentioned that, as a member of ACS, he never goes to their webpage but he reads their weekly newsletter. Perhaps a monthly newsletter from each IUPAC Division could be interesting reading for a very broad audience.

5. Update on Division membership

The list of newly appointed members and officers for 2018-2019 (see table at the end) was presented by RC and approved. The list includes their most recent e-mail contact details.

6. Finances of the Division

The total budget of Division VII for the biennium 2016 -2017 is: \$38,360. The amount spent so far is \$ 31,000 and attributed as follows: 2 projects of DDD, 2 projects of TRA and 1 project of NPU.

The budget allowed inviting Geok Bee Teh (Sharon) to the GA in Sao Paulo

There is enough money for 1 or 2 more projects if they can be submitted and approved by the end of the year 2017.

A new Interdivisional Committee was created on 'Green Chemistry and Sustainability'. Considering the fixed amount available for Divisions and Committees, the budget of the existing ones will be decreased accordingly as from the next biennium.

7. Update on Emeritus Fellows Program

Each subcommittee can name two candidates. As already decided in Copenhagen in 2016, RC will write a proposal to nominate J. Duffus. J. Fischer will nominate Toshi Kobayashi.

8. Updates from Subcommittees

A. Drug Discovery and Development (DDD)

TP gave a brief report in the absence of JF.

Books

The 3rd book on “Successful Drug Discovery”, edited by Janos Fischer, will be published later this year by Wiley. This series is most successful and will be continued next year. The royalties are paid to IUPAC. These are considered too low. Currently, they stand at 4%, while the standard is between 10-13%. Colin Humphris, Treasurer of IUPAC, later confirmed that the 4% profit is too low, considering the success and high demand for these books. The contracts will be reviewed by Lynn Soby, Executive Director, IUPAC Secretariat.

IUPAC-Richter Prize

JF mailed the following information: the composition of the Selection Committee for the 2018 IUPAC-Richter Prize has been sent to Lynn Soby. The prize giving will be organized in Nashville (USA) at the 36th NMCS (April 29 - May 2, 2018). JF is waiting for confirmation by the local organizer (Prof. Craig Lindsley, Vanderbilt University).

Projects

Project 2014-019-1-700. Novel Psychoactive Drugs of Abuse, chaired by V. Abbate. V Abbate reported that Part 1 of the manuscript describing synthetic cannabinoids was submitted to PAC 06/2017. Part 2 will be discussed during a special meeting of the project members in Sao Paulo. Terminology is a most difficult aspect when writing these articles. To illustrate this, VA evoked the term ‘abuse’. How do you define ‘abuse’? What concentration of a substance would qualify as abuse? Which compound would fall in the category of drugs that can then be classified as ‘abuse’?

Project 2003-044-1-700. Glossary of Combinatorial Chemistry Terms, chaired by A. Ganesan. This project had been dormant for many years, and now the current task force leader, Ganesan, reports that it is nearing completion.

B. Nomenclature for Properties and Units (NPU)

Activities in the Steering Committee on NPU

HMJ outlined the scope of the NPU founded in 1966. NPU is a patient-centered clinical laboratory terminology for use in the clinical laboratory sciences. Its function is to enable results of clinical laboratory examinations to be used safely across technology, time and geography. NPU terminology has been developed over 20 years and a Steering Committee has been established in collaboration with IFCC and the Danish Health Data Authority. One important goal is to establish NPU as an international standard for clinical use. The objectives of the Steering Committee is an agreement between SNOMED CT organisation and Steering Committee on NPU for future collaboration. New projects are set up to integrate all standards collected so far, such as in the field of molecular genetics, immunology.

HMJ provided summary slides that outlined the current progress of NPU and its Steering Committee. HMJ showed the content of a poster on the activities of NPU. This will be exhibited at the 46th IUPAC World Chemistry Congress held in Sao Paulo, 9 - 14 July 2017.

Colin Humphris gave some additional background information on the NPU project and explained why it is important to have such a system and why IUPAC is supporting the work.

HMJ gave a report about the progress made by the Steering Committee during the meeting held in Athens in June 2017.

Projects under the Subcommittee on NPU

Project "Urinary Calculi" (2001-070-1-700) chaired by G. Nordin.

Is closed down .

Project: "Establishing definitions for non-referenced terms in the NPU-terminology" (2010-035-2-700) chaired by H.Moller Johannessen: The working group has reviewed all the 3000 terms and following the work on qualifying the terms has been a process for many discussions - and is the reason for the delay in finalizing the project.

A Guideline for the managers of the NPU Terminology is ready in the first draft version and will be discussed in the forthcoming meeting in the C-SC-NPU in June 2017. The project is planned to be finalized by the end of 2017.

Project: "Molecular Diagnostics Revision"(IUPAC 2013-009-5-700) chaired by U.M.

Petersen. The project was scheduled to finalize in 2016. It has been delayed, in part because the field of molecular biology and its technology is developing extremely fast, causing continuous changes to both concepts and terminology, and enabling investigation of quite new patient properties. The project will be discussed in June 2017 in the IFCC-IUPAC (Sub)-Committee on Nomenclature for Properties and Units. We hope for acceptance of the metrological and terminological content, enabling us to finalize the project in 2017. HMJ reported that this project will be finalized very soon.

Project: The Mapping project (IUPAC 2006-008-1-700) chaired by Ulla Magdal Petersen

This first attempt at SCT mapping was stalled because of changes in the SCT concept structure. The Project cannot be completed as planned (because of recent changes in SNOMED CT), but will transfer the work product to 2014-017-1-700. The end date for the project is extended to 30-June-2016 in order to coincide with that of project 2014-017-1-700.

Project: Vocabulary for nominal properties and nominal examinations — basic and general concepts and associated terms (IUPAC 2004-023-1-700)

A version number 10 of the manuscript, hopefully the final version, will be submitted for publication in PAC in a few days.

The next meeting of the Subcommittee on NPU is scheduled to be held in Copenhagen in November 2017.

C. Toxicology and Risk Assessment (TRA)

In the absence of JD, RC reported the information given by JD.

Project 2009-034-2-700: "Risk Assessment of Effects of Cadmium on Human Health", chaired by Gunnar Nordberg

This project is close to completion. After a meeting of the core authors in June and revision by the project leader, G. Nordberg, the final draft of the paper has been submitted to PAC as a Technical Report following circulation to the authors to ensure that the final version is as accurate as possible.

Project 2011-032-1-700: "Concepts in Toxicology, Instructional Materials", chaired by Jane Huggins

This project has now been completed and the residual funds were allocated to defray the expenses of a meeting of the Working Group on Consolidation of the Glossaries of Terms Used in Toxicology.

Project 2013-001-1: "Glossary of terms used in Neurotoxicology and Reproductive/Developmental Toxicology", chaired by D. Templeton.

This project developed into 2 separate projects, one to prepare a glossary of terms used in neurotoxicology and the other to prepare a separate glossary of terms used in reproductive and developmental toxicology. Both projects have proceeded smoothly, and the Glossary of Terms used in Neurotoxicology has been published in Pure and Applied Chemistry as an IUPAC Recommendation. It has also been published in the Journal of Neurotoxicology in January of this year.

The "Glossary of Terms Used in Reproductive and Developmental Toxicology" has been revised to satisfy PAC reviewers and was accepted this week as an IUPAC Recommendation for publication in PAC.

Project 2013-006-1: "Preparation of a consolidated and extended IUPAC Glossary of Terms Used in Toxicology", chaired by J. Duffus.

A consolidated database of all current IUPAC approved toxicology terms has been compiled. All terms from the new glossaries resulting from project 2013-001-1 above have been included. All terms in the consolidated glossary were subject to revision where usage has changed or developed, or the wording is less clear than the working group or reviewers think it should be. Where necessary, new terms were added. A meeting was held in Tuebingen in November 2016 to deal with any outstanding problem and to carry out a final check before submitting the consolidated glossary to the RSC for publication in book form. It is hoped to make the final glossary available on the IUPAC website and in other ways online. Possibilities for a project or projects developing it further as an educational resource will be considered as well.

Project 2013-007-1-700: "Recent Advances in Nanoparticles and Colloidal Systems", chaired by V. Gubala.

VG reported that the project is completed and closed. It resulted in 2 articles on the verge of being published in PAC. A short version of the articles was published in Chemistry International, Volume 39, No.2, 2017, 10 – 13. It is entitled: Nanoparticles – On the brink of revolution? Or the endless pursuit of something unattainable? Authored by Emma Perkin and Vladimir Gubala.

Project 2013-023-1-700: "Toxicology in the Classroom II", chaired by W. Temple. Unfortunately this project has been inactive; TP will make a decision of how to proceed.

LJ reported on the Workshop she organizes in Mexico this year

9. New Projects

Approved

2016-044-2-700 "On-line dynamic NPU-manual", free online. Chair Y. B. L. Hansen

2016-045-2-700 "Safety of engineered nanomaterials". Chair L. Johnston

2017-012-1-700 "Glossary of terms in molecular toxicology". Chair D. Templeton

Under Review

presently none

Potential Submissions

DDD

1. H. Buschmann wants to write a proposal about decomposition of drugs.
2. M. Liebman intends to submit a proposal probably about translational medicine. He is expected to write a draft of a proposal that will be commented by JF and TP.
3. NC plans a symposium in Puerto Rico in 2019 entitled "A Survey of Neglected Diseases in South America". That might create the opportunity to conclude the so far unpublished Monge project. IUPAC money could come forward once major funding by other institutions is guaranteed. In any case, NC can apply for an IUPAC Div VII sponsorship.
4. JF intends to submit a new project for the continuation of his book series on 'Successful Drug Discovery'.
5. A.G. suggested a 'Glossary of terms in epigenetics' to clarify nomenclature.

NPU (HMJ)

1. On-line dynamic NPU manual, free online. Chair: Young Bea Lee Hansen
2. There are ideas to expand the definitions into fields, which are presently not represented. These include: Clinical Immunology, Clinical Microbiology, Functional Investigations, Educational Materials. There are, however, at present no definite project proposals in the pipeline, as volunteering for chairing projects is very limited. A model for fast projects would be welcome.

TRA

VA suggested a project on cathinones.

During the interdivisional meeting with Div VI (environment) in Busan, it was decided that the two divisions intend to cooperate on several projects.

Following topics were suggested:

1. JD (with P. Fedotov, Div VI) "Bioavailability and Bioaccessability of Metals". RC may also be interested.
2. VG has a project idea, which he wants to pursue with H. Garelick (Div VI) on "Nanomaterials, Environment and Human Health".
3. MS has suggested to P. Fedotov a project: "Chemistry and Sustainability". It would integrate the ideas of IUPAC president N. Tarasova.

TP said that the budget of Div VII would allow possible support for 1 or 2 of these 3 interdivisional projects. A possibility is to merge 2 & 3.

10. IUPAC Website: <https://iupac.org/>

The IUPAC secretariat now opens the way for the Divisions to handle themselves their data on the IUPAC-website. The site will be redesigned in the near future to attract new readers.

VG volunteered to be the liaison person for Division VII, working closely together with Fabienne Meyers. As VG masters the software of WordPress he is the right man to do so. He will enable a quick update of the data delivered by the members of Division VII.

11. Division VII rules (DT)

Doug Templeton went over the details of the existing Operating Procedures he wrote in 2009. Some parts were clarified. Some parts need to be updated. The document will be used by Richard Hartshorn, Secretary General, as a template for all Divisions. The updated copy will be available to all members shortly after the meeting.

12. Interdivisional Meetings

Session 1: 10:30-11:15h. Div VI (Environment) and VII

Session 2a: 11:30-12:15h. Div IV (Polymer) and VII

Session 2b: 11:30-12:15h. Div VII and VIII (Nomenclature)

Comments can be read in section 15 'Interdivisional Activities,, when applicable

13. Election for 2018-2019 Biennium (RC):

The list of the membership for the biennium 2018 – 2019 is given at the end of the minutes. The list was approved by the Council.

14. Meetings attended by members

15. Interdivisional Activities:

CCE

JD is not present and there is nothing to report

COCI

Nothing to report

ICGCSD (Interdivisional Committee on Green Chemistry for Sustainable Development)

MS reports through Skype: this committee has 5 TMs and lot of AMs. They are very active through Skype conferences. MS gave an overview how this subcommittee started and what is its rationale.

ISMC

C. Ober is stepping down as the subcommittee chair; VG will take the position for the next biennium.

ICTNS

RC could not attend their meetings because they were scheduled at the same time as our meetings. However, she was part of the meeting in the past and explained the role of ICTNS.

PAC

TP is the representative of the Division VII; Rita will become the representative of PAC as from 2018

Division I Physical and Biophysical Chemistry

LJ reported that there did not appear to be much interest in the Division VII nano-related projects from the Division I members that she contacted.

Division III Organic and Biomolecular Chemistry Division:

NC reports on the photochemistry congress, green chemistry in Africa/Latin America, on a series of glossaries in physical organic chemistry, on rules for abbreviation of protective groups, on several ongoing projects but nothing significantly overlapping. One potential project could be about ‘antibody-drug conjugates’, which is interesting for the Divisions III & VII because of its impact on human health.

Division IV Polymer

VG reports: Two projects were proposed – one related to the ‘Terminology and toxicology related to polymer degradation in the human body’; - the other was ‘Polymers and impact on human health’.

Division V Analytical

LJ discussed possible links between a new Division V project on analytical characterization of nanomaterials with Jan Lubuda, outgoing Chair of Div V. This project is cofounded by Div VII and LJ agreed to be part of the project team.

Division VI Environment

Nanopesticides are a potential project. Such a project overlaps with the engineered nanomaterial project. The agreement was to exchange information about their and our activities to find complementary projects. Further discussions between LJ and Sherine Obare focused on coordination between Division VI and VII projects on safety of nanomaterials. Discussion between LJ, TP and Rai Kookana resulted in strong support for developing a project before the end of the biennium.

Division VIII Chemical Nomenclature and Structure Representation

BP asked how to present the chemical compounds and their two or three dimension structures. With hydrogens, without hydrogens, wedge bonds, bold bonds etc. The questions were adequately addressed by the Div VIII President Karl-Heinz Hellwich and sparked vivid discussions but no specific project was identified.

16. Cooperation with Other Organizations

- ACS (TP) TP attends these meetings on a regular base
- AFMC (R. Hwu) to be determined
- EFMC (JF, ED) nothing to report
- ICSU (AK) there is no knowledge about present developments.
- IFCC (HMJ) NPU has a relationship with IFCC and a Steering Committee. C. Humphris will stay on the Steering Committee, in addition to his main task as treasurer of IUPAC
- IUTOX (JD) and NIH (JD) update from JD requested
- RSC (VG, AG) BMCS interaction with RSC from Ganesan – organization of conferences
- SOT (JD) nothing to report
- USNC (TP) part of National Academy of Sciences, meeting shortly, TP will represent
- WHO, WHO-IPCS (JD) nothing to report

17. Conferences of Interest for IUPAC Sponsorship

NC is part of the team that will organize the “2nd International Conference on Global Challenges in Neglected Tropical Diseases” June 25-27, 2018 in San Juan, Puerto Rico. The meeting is endorsed by IUPAC. NC might put Div VII on the leaflet.

18. Any additional business

Mustava Sozbilir, Chair of the "Committee on Chemistry Education", and Jan Apotheker, standing committee chairman, gave a brief overview of the Chemical Education projects and suggested a contribution to the project budget when applicable.

M. Sozbilir offered an option to participate in Young Ambassadors for Chemistry (YAK)-events and also in Flying Chemistry Educators Programs (FCEP).

19. Next Division meeting

The venue for the next Division Meeting will be Boston, USA, August 25-26, 2018. Hospitality will be given by Fabienne Meyers, Department of Chemistry, Boston University, Metcalf Center for Science and Engineering, 590 Commonwealth Ave, Boston, MA 02215, USA.

Membership IUPAC DIVISION VII
Chemistry and Human Health
2018-2019

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TM= Titular Member (up to 10), **AM** = Associate Member (up to 6), **NR** = National Representative (up to 10)