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Report to IUPAC Council on Division VIII Activities

It is a pleasure for me to report that the Division of Chemical Nomenclature and Structure Representation is supporting numerous projects and activities in our area of responsibility – Chemical Nomenclature, one of the core IUPAC activities, and probably the one which is most frequently associated with IUPAC.

Details on active projects can be found at http://www.iupac.org/nc/home/projects/projects-by-divisions/project-list-for-division.html?tx_wfqbe_pi1%5Bdivision%5D=Chemical%20Nomenclature%20and%20Structure%20Representation%20Division. Unfortunately this page is not always up to date and, more importantly, does not include nomenclature projects which have been assigned project numbers related to other divisions. Members of Division VIII have also been involved in projects administered through the Inorganic Chemistry Division, Organic and Biomolecular Chemistry Division, and Polymer Division, as well as the IUBMB-IUPAC Joint Commission on Biochemical Nomenclature (JCBN). The level of collaboration with other Divisions is both pleasing and functionally important (3 Division Committee members are also members of the Subcommittee on Polymer Terminology and 3 Division Committee members, besides the JCBN Chairman who is *ex officio* a member of our Division, are also Associate Members of JCBN), as work on nomenclature must necessarily progress through interactions of nomenclature specialists with discipline specialists. Division VIII looks forward to further cross-fertilisation of ideas and activities through these interactions.

Key project work includes further development of the International Chemical Identifier (InChI) and Preferred IUPAC Names (PINs). The Division has also been developing closer contacts with organisations which are or will be users of chemical nomenclature. Links with the International Organisation for Standardisation (ISO) resulted in a new project on developing nomenclature for carbon nanotubes and related nanomaterials. A scoping meeting earlier this year made it clear that also a collaboration on metal clusters is highly desirable.

The Division also operates an Advisory Subcommittee which we use as a way of communicating with our community of interest, in particular in relation to review of nomenclature proposals.

In the area of nomenclature, perhaps more than in others, we need to work hard to identify and fill with enthusiasm those with more than a spark of interest in the subject. This became particularly obvious when reviewing the few received nominations for the last TM elections. We welcome any suggestions and constructive comments on this issue.

Current Division Committee Membership

Dr. Karl-Heinz Hellwich (President)

Prof. Richard M. Hartshorn (Past President)

Dr. Ture Damhus (Secretary)

Titular Members: Dr. Michael A. Beckett, Prof. Philip Hodge, Prof. Alan T. Hutton, Prof. Risto S. Laitinen, Prof. Ebbe Nordlander, Prof. Amélia P. Rauter, Dr. Hinnerk Rey (Titular Members)

Dr. Kirill Degtyarenko, Prof. Md. Abul Hashem, Dr. Michelle M. Rogers, Dr. John B. Todd, Prof. Jiří Vohlídal, Dr. Andrey Yerin (Associate Members)

Prof. Vefa Ahsen, Prof. Dong Joon Choo, Dr. Gernot A. Eller, Prof. Wei Huang, Prof. Todd L. Lowary, Prof. József Nagy, Prof. Martin Putala, Mrs. Sumalee Tangpitayakul, Prof. Lidija Varga-Defterdarović (National Representatives)

Dr. Gerard P. Moss (Ex officio)

Division Elections

Election of officers and TMs for the 2016 – 2017 biennium has been completed. This process took rather longer than planned, partly because of delayed receipt of NAO nominations, technical problems with the submitted files and, in addition, inappropriate and incomplete nominations.

The Division VIII membership for the 2016 – 2017 biennium which will be submitted to the IUPAC Council for approval includes:

Dr. Karl-Heinz Hellwich (President)

Prof. Alan T. Hutton (Vice President)

Prof. Risto S. Laitinen (Secretary)

Prof. Osman Achmatowicz, Dr. Ture Damhus, Dr. Gernot A. Eller, Prof. Richard M. Hartshorn, Prof. Philip Hodge, Dr. John B. Todd, Prof. Jiří Vohlídal (Titular Members).

Dr. Michael A. Beckett, Dr. Michelle M. Rogers (Associate Members)

Dr. Andrey Yerin (National Representatives)

Dr. Gerard P. Moss (Ex officio)

We have yet to fill four Associate Member vacancies, and only when this has been done we will be able to appoint National Representatives (NRs) because NRs can come only from countries not already represented on the Division Committee. This means that their appointment has to wait until all other vacancies have been filled. However, given the low number of nominations we will not be able to fill all available NR positions.

Key Projects for 2014-2015

After the publication of the new Blue Book with some 1600 pages we look forward to completing the Brief Guides to the Nomenclature of Inorganic and Organic Chemistry in the near future.

The new Blue Book, *Nomenclature of Organic Chemistry, IUPAC Recommendations and Preferred Names 2013* was completed by Warren Powell with the help of a few Division Committee members and it was published right before Christmas 2013.

Unfortunately, there have already been a number of inconsistencies detected in the new Blue Book, so that we are currently trying to establish procedures for their solution and suitable publication as well as ways of communication in this context and last but not least measures in order to prevent similar situations for future projects. In the meantime the list of errata has reached the length of over 900 entries and we are looking for a suitable way of publication. The preparation of a corrected PDF of the book is intended. We have been in contact with the chair of ICTNS (Interdivisional Committee of Terminology, Nomenclature and Symbols) and

the IUPAC Secretariat in order to prevent similar situations for future projects. In addition to errors and inconsistencies which can be handled as errata we also identified some issues which require further study for which we intend to initiate a project potentially leading to a revised edition of this book.

We also anticipate significant progress being made on developing Preferred Names for inorganic compounds and for polymers. The document “Specifying the Coordination of Ligands to Central Atoms: Detailed Description of Grammar in the Kappa (κ) Convention” shall be a first step in this direction. Also the document “Preferred names of constitutional units for use in structure-based names of polymers” will be submitted for review before the end of this year.

Other projects nearing completion are the “Nomenclature of Flavonoids” which – after completion of public review and revision – will be resubmitted for publication soon, and the “Source-Based Nomenclature for Single-Strand Homopolymers and Copolymers” which will shortly be submitted to ICTNS via the Subcommittee on Polymer Terminology (SPT). After a long-lasting discussion over years between members of the Subcommittee on Polymer Terminology (SPT) and Division VIII on the basic approach of this document, a breakthrough was achieved only earlier this year which resulted in a new draft of the Source-based nomenclature clearly elaborating that source-based polymer names must be based on retained IUPAC names for monomers. In addition, only a limited number of frequently encountered polymer names have been included as “retained polymer names”.

Three new projects have been approved after the last General Assembly by the end of the last biennium:

- Implementation of InChI for chemically modified large biomolecules (2013-010-1-800)
- Nomenclature for metallacycles containing transition metals (2013-030-1-800)
- Structure-based Nomenclature for Regular Linear, Star, Comb and Brush Polymers (2013-031-3-800)

Project Reviews and New Funding Committed

Division VIII projects approved so far in this biennium are:

2013-056-1-800	Nomenclature of carbon nanotubes and related substances
2014-001-2-200	Terminology guidelines and database issues for topology representations in coordination networks, metal-organic frameworks and other crystalline materials
2014-003-2-800	End-of-line hyphenation of systematic chemical names
2014-034-2-400	Nomenclature for polymeric carriers bearing chemical entities with specific activities and names
2015-003-2-300	Nomenclature of Homodetic Cyclic Peptides Produced from Ribosomal Precursors
2015-019-2-800	Identifying International Chemical Identifier (InChI) Enhancements – QR codes and Industry Applications

Several other project proposals are in preparation. The Division has also been developing closer contacts with organisations that are, or will be, users of nomenclature. This includes project work with the International Union of Biochemistry and Molecular Biology (IUBMB) under the auspices of the Joint Commission on Biochemical Nomenclature (JCBN), and most recently with ISO.

International Organisation for Standardisation (ISO) Liaison

Links with the International Organisation for Standardisation (ISO) resulted in one of the above new projects (2013-056-1-800). The ISO Technical Committee (TC 229) working in this area has been conducting a selection process for experts to participate in IUPAC projects, together with nomenclaturists from Division VIII. It is anticipated that another project will be initiated on the development of nomenclature for metal clusters.

Subcommittee on the IUPAC International Chemical Identifier

The Division continues to support the development of the International Chemical Identifier (InChI) – one project has been funded so far this biennium. The Sub-Committee on the IUPAC International Chemical Identifier (InChI) is the body through which IUPAC maintains oversight of the scientific activities of the InChI Trust. It reports to Division VIII and to the Committee on Publications and Cheminformatics Data Standards (CPCDS, formerly CPEP).

Budget Report

The budget allocation to Division VIII for the current biennium is USD 70,400. According to IUPAC guidelines approximately 70 % (USD 49,280) of division budgets should be committed to support project work, and the remaining 30 % (USD 21,120) allocated to operational expenditure. As in past biennia in Division VIII we envision to exceed the operational expenditure target, because operational expenditure has been and will be used to support liaison activities (e.g. with the InChI Trust, ISO, ACS) which may lead to further future projects. There are also on-going commitments to support IUPAC involvement in the long-standing IUBMB-IUPAC Joint Commission on Biochemical Nomenclature (JCBN). According to the latest data I have, operational expenditure is just under USD 16,000, while further USD 18,650 have been committed to projects. Approximately USD 35,750 remain uncommitted. A number of project proposals are being formulated at present and I fully anticipate that most of the remaining funding will be allocated to new projects.

Publications Related to Div VIII since last report

Nomenclature of Organic Chemistry, IUPAC Recommendations and Preferred Names 2013 (The Blue Book), IUPAC; W. H. Powell, H. A. Favre (Eds.) XLIII, 1568 pp., IUPAC, Royal Society of Chemistry, Cambridge, UK, 2014

J. He, J. Chen, K.-H. Hellwich, M. Hess, K. Horie, R. G. Jones, J. Kahovec, T. Kitayama, P. Kratochvíl, S. V. Meille, I. Mita, C. dos Santos, M. Vert, J. Vohlídal, Abbreviations of polymer names and guidelines for abbreviating polymer names (IUPAC Recommendations 2014), *Pure Appl. Chem.* **86**(6), 1003 – 1015 (2014)

R. G. Jones, T. Kitayama, E. S. Wilks, R. B. Fox, A. Fradet, K.-H. Hellwich, M. Hess, P. Hodge, K. Horie, J. Kahovec, P. Kratochvíl, P. Kubisa, E. Maréchal, W. Mormann, C. K. Ober, R. F. T. Stepto, M. Vert, J. Vohlídal, Nomenclature and graphic representations for chemically modified polymers (IUPAC Recommendations 2014), *Pure Appl. Chem.* **87**(3), 307 – 319 (2015); Erratum: *Pure Appl. Chem.* **87**(4), 441 (2015)

G. J. Leigh, Polymer Nomenclature, *Chem. Int.* **35**(4), 25 – 26 (2013)

G. J. Leigh, The Special Case of Boron Hydrides, *Chem. Int.* **35**(5), 24 – 25 (2013)

G. J. Leigh, Use of Abbreviations, Enclosing Marks, and Line-Breaks, *Chem. Int.* **35**(6), 24 – 25 (2013)

A. Yerin, A. McNaught, S. Heller, InChI – The IUPAC International Chemical Identifier, Current Status and Future Development in Relation to IUPAC Activities, *Chem. Int.* **35**(6), 12 – 15 (2013)

By the time of the General Assembly in Busan, hopefully also the “Brief Guide to the Nomenclature of Inorganic Chemistry” will be published. Unfortunately, since the IUPAC journal *Pure and Applied Chemistry* has been contracted with the publishing house De Gruyter, we have been experiencing several problems. In this particular case, for example, IUPAC recommendations which have been described and followed in the manuscript have been disregarded during typesetting which made it necessary to repeatedly request sets of proofs. For other manuscripts the authors did not receive proofs at all, which resulted in errors introduced during copyediting carried through to the final printed version, and errors found in the ASAP publication were not corrected before printing – despite notification of the editors.



(Karl-Heinz Hellwich)

President

IUPAC Division of Chemical Nomenclature and Structure Representation