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Report to IUPAC Bureau on Division VIII Activities

It is my pleasure to report that the Division of Chemical Nomenclature and Structure Representation is supporting numerous projects and activities. Our area of responsibility – Chemical Nomenclature – is 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 (for a full list see below). Members of the Division 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). Such collaboration with other Divisions and also other organisations is essential and functionally important, because work on nomenclature must necessarily progress through interactions of nomenclature specialists with discipline specialists. So, three Division Committee members are also members of the Subcommittee on Polymer Terminology, and three Division Committee members (besides the JCBN Chairman who is an *ex officio* member of our Division Committee) are also Associate Members of JCBN. 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 early in 2015 made it clear that a collaboration on metal clusters is also highly desirable.

After the publication of the *Nomenclature of Organic Chemistry, IUPAC Recommendations and Preferred Names 2013* (the IUPAC Blue Book), a new project was initiated just recently to further develop the recommendations provided in this book.

A successful part of our work is dealing with the needs of the users. As an initiative for the International Year of Chemistry we started working on Brief Guides to several areas of Nomenclature. The first one on polymer nomenclature was run by the Subcommittee on Polymer Terminology and published three years ago as a two-page document.

The Brief Guide to the Nomenclature of Inorganic Chemistry has four pages and was published in issue 9 – 10/2015 of *Pure and Applied Chemistry* (DOI: 10.1515/pac-2014-

0718). The success of this publication can be judged from the fact that translations into several languages have already been completed. Further translations are in progress. A similar four-page Brief Guide to the Nomenclature of Organic Chemistry will hopefully be completed within this year. These Brief Guides should be thought of as quick references, and can easily be republished or included in Author Guidelines and textbooks. We already have a commitment from the authors of the widely used international textbook, "Inorganic Chemistry" by Housecroft and Sharpe, to reproduce the Brief Guide to the Nomenclature of Inorganic Chemistry in the new edition of their textbook to be published towards the end of this year.

In the meantime, we are well into the planning phase for the off-year meeting of the Division Committee. We thank the Royal Society of Chemistry (RSC) for kindly agreeing to host this meeting in Cambridge, UK. It is scheduled for August 4 – 5, 2016, with task group meetings to be arranged for August 1 – 3 (or on August 5 after the end of the Division Committee meeting), also giving us the possibility of interactions with the RSC, in particular the publishing division of the RSC, and the Cambridge Crystallographic Data Centre (CCDC).

Division Committee Membership 2016 – 2017

This biennium has again seen a significant changeover of membership. Current membership is as follows.

President: Dr. Karl-Heinz Hellwich

Vice President: Prof. Alan T. Hutton

Secretary: Prof. Risto S. Laitinen

Titular Members: Prof. Osman Achmatowicz, Dr. Ture Damhus, Prof. Philip Hodge, Prof. Robin Macaluso, Prof. József Nagy, Dr. Michelle M. Rogers, Prof. Jiří Vohlídal.

Associate Members: Dr. Michael A. Beckett, Prof. Ivan L. Dukov, Dr. Gernot A. Eller, Dr. Elisabeth Mansfield, Dr. Keith T. Taylor.

National Representatives: Dr. Fabio Aricó, Prof. Hyo Won Lee, Prof. Todd L. Lowary, Prof. Ebbe Nordlander, Prof. Martin Putala, Prof. Amélia Pilar Rauter, Jan Pieter van Lune, Andrey Yerin.

Ex officio: Dr. Gerard P. Moss, Prof. Richard M. Hartshorn.

This leaves us with one AM vacancy and two NR vacancies which we are going to try to fill with suitable candidates.

Division Elections

Election of TMs for the 2016 – 2017 biennium 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. Also the remaining vacancies result from the low number of nominations received.

It is obvious that in the area of nomenclature, perhaps more than in others, we need to work hard to identify colleagues with more than a spark of interest in the subject – and more so, to motivate and fill them with enthusiasm to spend their time and effort as volunteers into the goals of our Division and Union. We welcome any suggestions and constructive comments on this issue.

Projects in the final stages of preparation

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 – after completion of review and revision – will be submitted for publication by March 2016. 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 last 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”. Also the document “Preferred names of constitutional units for use in structure-based names of polymers” will be resubmitted for publication during the next few weeks.

Publications

For a list of publications related to Division VIII during the period 2014 – 2015 see below.

Since the IUPAC journal Pure and Applied Chemistry has been contracted with the publishing house De Gruyter, we have unfortunately been experiencing several problems. For example, there have been several IUPAC recommendations which have been described and correctly used in the manuscripts, but which have been disregarded during typesetting. This made it necessary to repeatedly request further revision and renewed proofreading. For other manuscripts the authors did not receive any proofs, which resulted in errors that were introduced during copyediting being carried through to the final printed version. The errors found in the ASAP online publications were not corrected before printing – although the editors were notified. However, these problems were raised with the De Gruyter representatives at the GA in Busan, and were also discussed there at the meeting of the PAC Editorial Advisory Board. Assurances were obtained that these problems were associated with the introduction of a new publishing platform and were not like to happen again.

Project Reviews and Funding Committed

Division VIII projects approved in the 2014 – 2015 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
2015-035-2-800	Continuation of the revision of IUPAC recommendations on carbohydrate nomenclature [Project extension]
2015-052-1-800	Corrections, revisions and extension for the <i>Nomenclature of Organic Chemistry - IUPAC Recommendations and Preferred Names 2013</i> (the IUPAC Blue Book)
2015-053-1-200	Survey of definitions and use of common solid-state chemistry Definitions

In addition, another project proposal has been reviewed, and has been resubmitted in revised form earlier this year. This project proposal is ready for approval:

2015-025-2- McEwen: InChI extension for mixture composition.

Further project proposals are in preparation or under consideration. 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.

Subcommittee on the IUPAC International Chemical Identifier

The Division continues to support the development of the International Chemical Identifier (InChI). The Subcommittee on the IUPAC International Chemical Identifier is the body responsible for the scientific activities supported by the InChI Trust. It reports to Division VIII and to the Committee on Publications and Cheminformatics Data Standards (CPCDS, formerly CPEP). One new project has recently been funded and started by the end of the last biennium. Another one was reviewed and is – after revision – now ready for approval (see proposal 2015-025-2- above).

Advisory Subcommittee

Division VIII 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.

Unfortunately, we are still facing technical problems with the Discussion Board – a means of communication and file exchange between Division Committee members and also with the Advisory Subcommittee members – and the IUPAC web site. We hope that these communication tools will be updated in the near future in order to facilitate our work.

International Organisation for Standardisation (ISO) Liaison

We have had a liaison with the International Organisation for Standardisation (ISO) for the past couple of years. This resulted in one of the above mentioned new projects (2013-056-1-800) aiming at developing nomenclature for carbon nanotubes and related nanomaterials. The project task group just recently had a very productive meeting on February 23rd, 2016, in Würzburg, Germany. The ISO Technical Committee (TC 229) working in this area had been conducting a selection process for experts to participate in IUPAC projects together with nomenclature experts from Division VIII. It is anticipated that another project will be initiated on the development of nomenclature for metal clusters.

Budget Report

Some 96 % (~ USD 67,900) of the budget for the last biennium were spent by the end of the last biennium, which is mainly attributed to the fact that at the end of the year the exact amount of remaining budget was not totally clear.

The biennial budget allocation to Division VIII for the new biennium is unchanged (USD 70,400). According to IUPAC guidelines approximately 70 % (USD 49,280) of the Division budget should be committed to support project work, and the remaining 30 % (USD 21,120) allocated to operational expenditure. As in past biennia (except the just terminated biennium) in Division VIII we expect 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).

No commitments have been made and no operational expenses spent so far this year.

Key Projects for 2016 – 2017

Providing a standardised naming of chemical compounds for international communications on chemistry was the origin of IUPAC. In more recent times, the recognition that ever increasing interdisciplinarity, resulting in the boundaries between the disciplines becoming more and more blurred, led to the creation of Division VIII in 2002. The aim was to concentrate the nomenclature activities and to unify the recommendations so as to allow IUPAC to speak with one voice. These activities of our Division will be intensified as they are clearly covered by the Mission Statement in the new strategic plan ("The International Union of Pure and Applied Chemistry is the global organization that provides objective scientific expertise and develops the essential tools for the application and communication of chemical knowledge for the benefit of humankind and the world."). In general, the importance of nomenclature should be more strongly emphasised in IUPAC publications.

Similarly, it was noticed quite a while ago – already during the General Assembly in San Juan 2011 – that also in the area of terminology IUPAC should go a step forward in unifying definitions of terms beyond the restricted areas of disciplines. A recent meeting at the end of 2015 between members of Division VII and the President of Division VIII towards this goal prepared the way for a cross-Divisional project with this aim.

Initiatives towards the goal of unified nomenclature recommendations, as already exemplified with projects mentioned above, will be intensified. One example is the new project on "Corrections, Revisions and Extension" for the new Blue Book. Unfortunately, since its publication over two years ago quite a number of errors and inconsistencies have been detected in the more than 1600 pages of this book. The list of errata which has been prepared, and still is being amended on a regular basis, is publicly available on the IUPAC nomenclature homepage run by Gerry Moss and hosted at the University of London (<http://www.chem.qmul.ac.uk/iupac/bibliog/BBerrors.html>). In the meantime it has grown to contain more than 1000 entries. In addition to errors and inconsistencies which can be handled as errata, the task group has already identified sections which require further study, potentially leading to revision or addition of sections. The aim is not only to produce a corrected PDF of the Blue Book but eventually also to prepare a revised printed edition. This revision will include sections which were omitted in the 2013 edition, and revisions of sections which either are not consistent with other sections within the book or may be made more user-friendly if revised. Such revisions could be simplifications, or the removal of alternatives, or better alignments with other IUPAC recommendations such as the Red Book, the Purple Book and Biochemical Nomenclature.

This project will hopefully in the near future be supplemented by an interdivisional project on a revision and extension of one of the most frequently downloaded PAC documents: the "Glossary of class names of organic compounds and reactive intermediates based on structure" [*Pure Appl. Chem.* **67**, 1307 – 1375 (1995)].

In addition to work on projects, measures need to be established in order to ensure that similar embarrassing situations as those described for the Blue Book (but also with a few other recent IUPAC Publications in *Pure Appl. Chem.*) will not happen again in future projects. This will

include collaboration with the Interdivisional Committee of Terminology, Nomenclature and Symbols (ICTNS) and the other Divisions. A part of this initiative will comprise the review and potential revision of review procedures and also the removal of pressure by strict deadlines from the many volunteers – in particular pressure by publishers.

Beyond the classical methods of nomenclature a few areas have already been identified in which we need to think and develop concepts for the rational and unambiguous description of structures with ever increasing sizes which are accessible by new developments of synthetic procedures and required by advances in analytical methods characterising for example supramolecular structures.

As briefly mentioned above, we are reaching out to our users. This will include contacts with other organisations – and has already led to the above mentioned joint project with ISO. Contacts are also being sought with the Cambridge Crystallographic Data Centre (CCDC) and the European Patent Office. Joint workshops on nomenclature are being considered together with the ACS and the RSC. In addition, Division Committee members are actively presenting IUPAC documents in the form of posters or reprints of the Brief Guides at relevant conferences or congresses.



(Karl-Heinz Hellwich)

President

IUPAC Division of Chemical Nomenclature and Structure Representation

Appendix 1: Publications Related to Division VIII during the last biennium**a) Recommendations**

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)

R. M. Hartshorn, K.-H. Hellwich, A. Yerin, T. Damhus, A. T. Hutton, Brief Guide to the Nomenclature of Inorganic Chemistry, *Pure Appl. Chem.* **87**(9 – 10), 1039 – 1049 (2015); reprinted as a four-page tear-off document in the centre of *Chem. Int.* **37**(5 – 6) (2015).

b) Other publications

R. Bucat, Visualization, Mental Models, and the "Reality", *Chem. Int.* **36**(1), 9 – 13 (2014)

J. Meija, Symbols of the Elements, *Chem. Int.* **36**(1), 20 – 21 (2014)

In Memoriam: Henri A. Favre 1926 – 2013, *Chem. Int.* **36**(2), 17 – 18 (2014)

J. Meija, Symbols of the Elements, Part II, *Chem. Int.* **36**(3), 18 – 20 (2014)

J. Meija, Symbols of the Elements, Part III (concluded), *Chem. Int.* **36**(4), 25 – 26 (2014)

E. Scerri, On the Naming and Symbols for Elements 115 and 112, *Chem. Int.* **36**(4), 26 – 27 (2014)

New Edition of the "IUPAC Blue Book" Nomenclature of Organic Chemistry – IUPAC Recommendations and Preferred Names 2013, *Chem. Int.* **36**(4), 22 (2014)

I. Mills, On the Use of Italic and Roman Fonts for Symbols in Scientific Text, *Chem. Int.* **36**(5), 23 – 24 (2014)

Mark I. Borkum, Jeremy G. Frey, What's in a Name? Quite a Lot, as it Happens! *Chem. Int.* **37**(2), 7 – 9 (2015)

Evan Hepler-Smith, The History of the IUPAC Nomenclature of Organic Chemistry, *Chem. Int.* **37**(2), 10 – 14 (2015)

Appendix 2: Currently active Division VIII projects

Number	Chair	Short Title	Comments
2001-081-1-800	(Kahovec) Fradet	Nomenclature for Dendrimers	
2003-042-1-800	(Kitayama) Jones	Source-Based Polymer Nomenclature	Resubmitted
2003-045-3-800	Town	Graphic Representation Standards	see 2012-033-1-800 below
2004-024-1-800	Moss	JCBN Cyclic Peptides	Revive
2006-019-1-800	(Dixon †) Moss	JCBN Phosphorus Compounds	Revive
2006-038-1-800	Hartshorn	Inorganic PINs/Kappa Convention	
2009-018-2-800	Rauter	JCBN Flavonoids Nomenclature	Resubmit
2009-022-2-800	(Cammack) Ennis	JCBN biologically important Small Molecules	
2009-040-2-800	Batchelor	InChI Organometallic Compounds	
2009-041-1-800	Goncharoff	InChI Markush Structures	
2009-042-1-800	Yerin	InChI Polymers	
2009-043-2-800	Grethe	InChI Reactions	
2010-055-1-800	Hartshorn	Inorganic and Organic Brief Guides	
2011-035-1-800	Jones	Inorganic Polymers (TINCOPS)	
2011-044-1-300	Brimble	Abbreviations for Protecting Groups	Completed, Errata needed
2012-023-2-800	Nicklaus	InChI Tautomerism	
2012-033-1-800	Town	Graphic Representation of Reactions	Extension needed
2012-037-1-800	Yerin	Hydrogenation (Hydro Prefixes/Indicated H)	
2012-039-2-800	Vliegenthart	JCBN Carbohydrate Nomenclature	Extended, see below
2012-045-1-800	Beckett	Boron Nomenclature	
2012-046-2-800	(Rey)	InChI Inorganic	Transfer to new Chair
2013-010-1-800	Taylor	InChI Biomolecules	
2013-030-1-800	Hutton	Metallacycles	
2013-031-3-800	Chen	Star Polymers	
2013-039-2-300	Blackburn	Phosphoryl Transition States	
2013-056-1-800	Mansfield	Carbon Nanotubes	
2014-001-2-200	Öhrström	Topology of Metal-Organic Frameworks	
2014-003-2-800	Dijkstra	Hyphenation of Chemical Names	
2014-034-2-400	Vert	Polymeric Carriers	
2015-003-2-300	Reaney	Homodetic Cyclic Peptides	
2015-019-2-800	Hartshorn	InChI QR-Code Extension	
2015-035-2-800	Vliegenthart	JCBN Carbohydrates [Project extension]	
2015-052-1-800	Hellwich	Blue Book Extension and Revision	
2015-053-1-200	Macaluso	Solid State Terminology	
2006-004-1-400	He	Abbreviations for Polymer Names	Completed, Errata needed
2008-015-1-400	Mormann	Preferred Names for Polymers	revise and resubmit
2008-020-1-400	Hodge	Web Guide to Polymer Naming	prepare final draft
2009-047-1-400	Hellwich	Stereo Poly	draft ms.
2014-033-1-400	Vert	Lactic Acid [Project extension]	
2015-025-2-	McEwen	InChI Mixtures	approve