

Division VIII

Chemical Nomenclature and Structure Representation

Report to IUPAC Bureau, Bratislava, April 2018

Submitted by Prof Alan Hutton, Division President

I. Highlights/Executive Summary

The activities of Division VIII are closely aligned with IUPAC's Mission Statement, namely to "provide objective scientific expertise and develop the essential tools for the application and communication of chemical knowledge for the benefit of humankind and the world."

Several new projects have been initiated and approved since the last report, of which one (*Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature*) has already produced a draft report of some significance, in that this project provides overarching recommendations that now allow completion of several projects in different states of progress. One such longstanding project (*Boron hydride nomenclature*) has since been finalised and submitted to ICTNS for review, and it is expected that the other projects mentioned in Section III below will now be more rapidly concluded.

Other key priorities are to initiate a new edition of "The Red Book" (*Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005*), continue with the revision and further development of the recommendations in "The Blue Book" (*Nomenclature of Organic Chemistry, IUPAC Recommendations and preferred names 2013*), finalise and publish the organic version of the Brief Guides series, as well as several other projects that are nearing completion, as highlighted in Section III.

Continued collaboration with the International Organisation for Standardisation (ISO) will take place in initiating a project working towards appropriate nomenclature for nanoparticles, and our support for the work of the InChI Subcommittee is ongoing.

The next meeting of the Division Committee, along with various Task Group Meetings, will be over the period 10–14 August 2018 in Basel, Switzerland.

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

Probably the most significant recent advance, right at the end of the last biennium, was the draft report of the *Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature* project, details of which are given in Section III (below). As a result of this three-day meeting in London in November 2017, the basis has been laid for the completion of several interlinked projects, as several overarching principles were established in that meeting (and in subsequent discussion) that should now enable rapid progress. Already the boron hydride nomenclature project has been submitted to ICTNS, and a priority for this biennium will be to apply the outcomes of that meeting to complete the projects on metallacycle nomenclature, preferred names for inorganic compounds (this means

primarily the specification of ligating atoms in coordination compounds – the kappa document), and the Blue Book extension and revision.

A key project to initiate in this biennium, and which will extend well into the next biennium, is to publish a new, updated version of “The Red Book”, *Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005*. This will be a major undertaking and the Task Group Chair and Members will have to be chosen with care. Completely new chapters on solids, boron hydrides, organometallic compounds and other topics are envisaged; fortunately several currently extant projects will feed directly into the new book. This endeavour will probably be funded initially as several smaller projects, culminating in a final project to compile and edit the final book. We hope to have a draft plan for this major undertaking in place before this year’s Division Committee Meeting.

Priority will be given to work on the revision of “The Blue Book” (*Nomenclature of Organic Chemistry, IUPAC Recommendations and preferred names 2013*). Thus far the work on systematically collating the list of corrections has revealed further areas where additional discussion, unification and even extension are needed. Some of these matters have already been given a sound basis by the discussions, agreements and decisions made during the Alignment Project meeting in London in November 2017.

We have had a liaison with the International Organisation for Standardisation (ISO) for the past couple of years. This resulted in a project (2013-056-1-800) which produced a first draft with approaches towards a nomenclature for carbon nanotubes and related nanomaterials. The project task group is composed of experts in the area selected by the ISO Technical Committee (TC 229) working in this area and nomenclature experts from Division VIII. It is a priority for this biennium to pursue this liaison further, and to initiate a project on the development of nomenclature for nanoparticles, an area of significant importance for ISO. Initially, it is proposed that a project on metal cluster nomenclature be initiated, to see if this can be extended to nanoparticles. The conclusion of the scoping meeting with ISO representatives in London in 2015 was that such nomenclature may well have to be InChI-based.

Several long-running projects are nearing completion (these are itemised in Section III, below) and it will be a priority in this biennium to bring these to a conclusion.

The off-year Division Committee Meeting is planned to be held in Basel, Switzerland, on 13 and 14 August 2018, with Task Group Meetings being held over the preceding three days (10–12 August). We are also starting to plan for the GA in Paris in 2019 and have established the need for funding for the InChI Subcommittee to meet there, as it has been more than eight years since they last met as a formal committee.

III. Overall report of Division activities and achievements during 2016-2017 biennium organized by the Goals and Objectives laid out in the current IUPAC Strategic Plan

GOALS

Provide scientific expertise to address critical world needs

A full list of currently active projects can be found in Section IV (below). These provide the scientific expertise to name chemical substances – whether this addresses a critical world

need is debateable, but it is certainly at the core of IUPAC activities, and is most likely the one most frequently associated with IUPAC. Certainly, for the international exchange of goods, and in particular chemicals, an unambiguous and global nomenclature and classification is a critical requirement for transportation and import/export authorities.

Since the last report several **new projects** have been initiated and approved:

- *Revision and integration of the carbohydrate related recommendations on Glycoconjugates and Glycoinformatics* (Chair: Vliegenthart). This is an extension of a previous project which has made substantial progress, but the extent of the undertaking was clearly underestimated in the original proposal and there are currently several strands which need to be drawn together to provide an authoritative, integrated and overarching document.

- *Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature* (Chair: Hellwich). This project intends to provide the basis for completion of several projects with different states of progress:

- Boron hydride nomenclature (2012-045-1-800)
- Metallacycles nomenclature (2013-030-1-800)
- Preferred names for inorganic compounds (kappa document) (2006-038-1-800)
- Blue Book revision and extension (2015-052-1-800)

by reaching a consensus on

- the grouping of substituents or ligands with different kinds of modifications
- the alphabetical order of substituents or ligands with different kinds of modifications
- the positioning of locants in chemical names
- the positioning of kappa terms in chemical names

The project comprised one meeting held in London in November 2017 and has thus far resulted in a draft report; the intention is to publish an article in *Chemistry International* and possibly a Recommendation in PAC. Already a successful outcome of the project is that as a result of the decisions made at the meeting the document on boron hydride nomenclature could be finalised and has now been submitted to ICTNS for review.

- *Graphical representation standards for chemical reaction diagrams* (Chair: Taylor). This project will provide a single, comprehensive set of guidelines for creating chemical reaction diagrams in printed and in electronic media. The recommendations will incorporate and complement previous IUPAC projects on graphical representation standards.
- *Graphical representation of polymer structures* (Chair: Hellwich). This project intends to provide a single and comprehensive set of guidelines for the graphical representation of polymer structures, again incorporating and complementing the work done in previous projects.

Several projects are in the **final stages** of preparation:

- *Boron hydride nomenclature*. As mentioned above, as a result of the Alignment Project meeting in London in November 2017 this document has been finalised and submitted to ICTNS for review.
- *Nomenclature of Flavonoids*. The second set of page proofs has been checked, but the number and nature of corrections to be done by the typesetter will require another set of proofs before the document can finally be published.
- A document on *Nomenclature and terminology of dendrimers and hyperbranched polymers* has undergone review by ICTNS and the public. The revised version needs only a final check before being submitted for publication.
- *Hyphenation of chemical names*. This document, which addresses the needs expressed in discussions with De Gruyter's production department, is being finalised for Division review.
- *Inorganic and organic Brief Guides*. The inorganic Brief Guide was published in 2015 and the organic version is nearly complete.
- *Nomenclature and terminology for lactic acid-based polymers* (administered through Division IV) is about to be submitted for review by ICTNS and the public.
- *A concise guide to polymer nomenclature for authors of papers and reports in polymer science and technology* (administered through Division IV) is close to submission for ICTNS and public review.

The following projects were **completed** during the last biennium:

- *Source-based nomenclature for single-strand homopolymers and copolymers* (IUPAC Recommendations 2016), *Pure Appl. Chem.* **88**(10 – 11), 1073 – 1100 (2016).
- *Comprehensive glossary of terms used in toxicology* (a Division VII project) contains a nomenclature appendix edited by Division VIII members.
- *Preferred names of constitutional units for use in structure-based names of polymers*. Published in PAC in November 2017 (see list of publications in Section IV).

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). This activity addresses the critical world need for chemical information to be codified and digitized.

Increase the value of our products and services

By condensing the essential elements of chemical nomenclature into the “Brief Guides” (Polymer, Inorganic, and soon to be completed Organic), we are increasing the value of our efforts in nomenclature by making them available in simplified form to students and authors. Revisiting and revising existing IUPAC nomenclature principles and rules as the science of chemistry develops and new systems are discovered clearly increases the value of our endeavours.

Improve the vitality, effectiveness and efficiency of our Union

One aspect of efficiency is certainly if new project task groups and in particular task group chairs familiarise themselves with relevant existing IUPAC guidelines and recommendations and apply them early on in new drafts. The goal must be consistency and uniformity between the different disciplines within chemistry and IUPAC.

OBJECTIVES

Brand IUPAC in the minds of stakeholders

and

Improve quality and frequency of communication with stakeholders

Several of the publications listed in Section IV (below) are in *Chemistry International* and provide communication channels both within the IUPAC community and to the larger stakeholder base. Often the articles in *Chemistry International* trigger users to consult the latest Recommendations as published in PAC, or to turn to the latest edition of any of the “Colour Books”.

Distribution of the “Brief Guides” at conferences and to students and schools and universities, either in hard or electronic copy, also fulfils this objective, as does the presentation of posters on nomenclature at conferences – this has been done recently for both the Inorganic Brief Guide and Boron Hydride projects. Our objective of having publishers reproduce the “Brief Guides” in their text books is slowly being realised, and Pearson has recently agreed to include the Inorganic Brief Guide as a fold-out in the upcoming 5th edition of *Inorganic Chemistry* by Housecroft and Sharpe.

Division VIII is currently supporting and contributing to the budget of two International Year of the Periodic Table projects which will contribute strongly to IUPAC branding and communication.

Increase revenue

No input here unless IUPAC receives royalties from the sale of our “Colour Books”. Some revenue may be realised indirectly by our distribution of the “Brief Guide” series which references (with hyperlinks) the IUPAC publications.

Expand and retain member and volunteer base with an emphasis on diversity and inclusion

The current Division VIII Committee (see table of membership in Section IV below) of 26 elected or appointed members comprises 16 males and 10 females (TMs: 7 male, 3 female; AMs: 3 male, 3 female; NRs: 6 male, 4 female) and there is a reasonable geographical spread, though amongst the TMs and AMs the members are mainly based in Europe or the USA. This is probably a reflection of where the expertise in chemical nomenclature has traditionally resided, and efforts must be made to recruit and train members from, in particular, the Far East, Australasia, South America and Africa. We are fortunate to have Committee Members not only from academia, but also from research institutions, the industrial sector, as well as CAS and CCDC.

Enhance interdivisional interaction and collaboration

Members of Division VIII have 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. Currently several Division VIII Committee members are also members of the Subcommittee on Polymer Terminology, others are involved in projects administered through Division IV, and three Division VIII Committee members (besides the JCBN Chairman who is an *ex officio* member of our Division Committee) are also Associate Members of JCBN. There is also cross-membership with Division III. Division VIII looks forward to further cross-fertilisation of ideas and activities through these interactions.

Most recently an initiative has been started towards a closer collaboration with CPCDS because of the overlap of interests and responsibilities in the area of structure representation. In this regard an initiative to develop jointly a Unicode character set for chemistry has been proposed to CPCDS.

Emphasize multidisciplinary projects addressing critical global issues

Further development of the International Chemical Identifier (InChI) involves computer scientists and information specialists. 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 challenging and yet promising project on developing nomenclature for carbon nanotubes and related nanomaterials. Preparations for another project with a similar collaboration on metal clusters are under way. Recently established contacts with the Cambridge Crystallographic Data Centre (CCDC) and the European Patent Office offer further avenues for multidisciplinary projects.

Support chemistry education, particularly in developing countries

The Brief Guide to the Nomenclature of Inorganic Chemistry has four pages and was published in *Pure and Applied Chemistry* in October 2015. It is aimed at advanced high school pupils or early undergraduate students, as well as a handy reference for postgraduate researchers. Its success can be judged from the fact that translations of this document into several languages have already been completed. Reprints and posters have also been prepared for distribution and presentation at relevant conferences or congresses. The publishing house Pearson has agreed to include it as a fold-out in the upcoming 5th edition of *Inorganic Chemistry* by Housecroft and Sharpe.

A similar four-page Brief Guide to the Nomenclature of Organic Chemistry is in the final stages of completion. These Brief Guides should be thought of as quick references, and can easily be republished or included in Author Guidelines and textbooks.

Division VIII is currently supporting and contributing to the budget of two International Year of the Periodic Table projects which will have obvious impact on chemistry education.

Acknowledgement

The help and advice of current Division VIII Past-President Karl-Heinz Hellwich and Division Secretary Risto Laitinen in the compilation of this report is gratefully acknowledged.

IV. Tabular material

1. DIVISION VIII MEMBERSHIP 2018 – 2019

Name	Status	Term	NAO
Prof. Alan T. Hutton	President	2018-2021	South Africa
Prof. Risto S. Laitinen	Secretary	2016-2019	Finland
Dr. Karl-Heinz Hellwich	Past President	2018-2019	Germany
Prof. Michael A. Beckett	TM	2018-2019	United Kingdom
Prof. Edwin Constable	TM	2018-2019	Switzerland
Dr. Ture Damhus	TM	2018-2019	Denmark
Prof. Robin T. Macaluso	TM	2018-2019	USA
Prof. Ebbe Nordlander	TM	2018-2019	Sweden
Prof. Amélia Pilar Rauter	TM	2018-2019	Portugal
Dr. Michelle Monnens Rogers	TM	2018-2019	USA
Dr. Elisabeth Mansfield	AM	2018-2019	USA
Prof. József Nagy	AM	2018-2019	Hungary
Molly A. Strausbaugh	AM	2018-2019	USA
Dr. Keith T. Taylor	AM	2018-2019	USA
Dr. Clare A. Tovee	AM	2018-2019	United Kingdom
Prof. Jiří Vohlídal	AM	2018-2019	Czech Republic
Dr. Fabio Aricò	NR	2018-2019	Italy
Prof. Neil Burford	NR	2018-2019	Canada
Prof. Ana Maria da Costa Ferreira	NR	2018-2019	Brazil
Prof. Safiye Erdem	NR	2018-2019	Turkey
Prof. Sangho Koo	NR	2018-2019	Korea
Dr. Erik Szabo	NR	2018-2019	Slovakia
Prof. Rafał Kruszyński	NR	2018-2019	Poland
Dr. Ladda Meesuk	NR	2018-2019	Thailand
Dr. Maria A. Petrova	NR	2018-2019	Bulgaria
Andrey Yerin	NR	2018-2019	Russia
Dr. Gerard P. Moss	<i>Ex Officio</i>	2016-2019	United Kingdom
Prof. Richard M. Hartshorn	<i>Ex Officio</i>	2016-2019	New Zealand
	10 TMs, 6 AMs, 10 NRs		

as of 1 January 2018

2. CURRENTLY ACTIVE DIVISION VIII PROJECTS

Number	Chair	Short Title	Comments
2001-081-1-800	(Kahovec) Fradet	Nomenclature for Dendrimers	in Revision, to resubmit
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) Damhus	Inorganic PINs/Kappa Convention	
2009-018-2-800	Rauter	JCBN Flavonoids Nomenclature	in 2nd Proof-read
2009-022-2-800	(Cammack/Ennis)	JCBN biologically important Small Molecules	Transfer to new Chair
2009-040-2-800	Batchelor	InChI Organometallic Compounds	
2009-041-1-800	Goncharoff	InChI Markush Structures	no feedback
2009-042-1-800	Yerin	InChI Polymers	
2009-043-2-800	Grethe	InChI Reactions	
2010-055-1-800	Hartshorn	Inorganic and Organic Brief Guides	Part 1 completed, part 2 nearly
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	see 2017-036-2-800 below
2012-037-1-800	Yerin	Hydrogenation (Hydro Prefixes/Indicated H)	
2012-039-2-800	Vliegenthart	JCBN Carbohydrate Nomenclature	see 2015-035-2-800 below
2012-045-1-800	Beckett	Boron Nomenclature	Divisional review
2012-046-2-800	(Rey)(Hartshorn)	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	finalise for submission
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	finalise for review
2014-034-2-400	Vert	Polymeric Carriers	
2015-003-2-300	Reaney	Homodetic Cyclic Peptides	
2015-019-2-800	Hartshorn	InChI QR-Code Extension	
2015-025-4-800	McEwen	InChI Mixtures	
2015-035-2-800	Vliegenthart	JCBN Carbohydrates [Project extension]	see 2017-026-1-800 below
2015-052-1-800	Hellwich	Blue Book Extension and Revision	
2015-053-1-200	Macaluso	Solid State Terminology	
2017-026-1-800	Vliegenthart	JCBN Carbohydrates [Project extension]	
2017-033-1-800	Hellwich	Alignment of Nomenclature Principles	draft report
2017-036-2-800	Taylor	Graphic Representation of Reactions	
2017-039-2-800	Hellwich	Graphic Representation of Polymers	
2006-004-1-400	He	Abbreviations for Polymer Names	Completed, Errata needed
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]	immediate submit to ICTNS

3. PUBLICATIONS RELATED TO DIVISION VIII SINCE LAST GA (SAO PAULO, AUGUST 2017)

Recommendations

G. M. Blackburn, J. Cherfils, G. P. Moss, N. G. J. Richards, J. P. Waltho, N. H. Williams, A. Wittinghofer, How to name atoms in phosphates, polyphosphates, their derivatives and mimics, and transition state analogues for enzyme-catalysed phosphoryl transfer reactions (IUPAC Recommendations 2016), *Pure Appl. Chem.* **89**(5), 653 – 675 (2017)

W. Mormann, K.-H. Hellwich, J. Chen, E. S. Wilks, Preferred names of constitutional units for use in structure-based names of polymers (IUPAC Recommendations 2016), *Pure Appl. Chem.* **89**(11), 1695 – 1736 (2017).

J. Duffus, D. M. Templeton, M. Schwenk, *Comprehensive Glossary of Terms Used in Toxicology*, Royal Society of Chemistry, 2017 (contains a 35 pages appendix of systematic names for drugs and agrochemicals, thoroughly corrected by the President of Division VIII).

Other publications

J. Reedijk, On the Naming of Recently Discovered Chemical Elements — the 2016 Experience, *Chem. Int.* **39**(2), 30 – 32 (2017).

R. Weir, IUPAC Standards and Recommendations, *Chem. Int.* **39**(2), 34 – 35 (2017).

R. Boucher, S. Heller, A. McNaught, The Status of the IUPAC InChI Chemical Structure Standard, *Chem. Int.* **39**(3), 47 (2017).

R. C. Hiorns, A Personal View of the Life and Times of the Subcommittee on Polymer Terminology, *Chem. Int.* **39**(4), 14 – 19 (2017).

L. Mc Ewen, InChI'ng forward: Community Engagement in IUPAC's Digital Chemical identifier, *Chem. Int.* **40**(1), 27 – 30 (2018).

K.-H. Hellwich, K.-M. Roy, Herkunftsbezogene Nomenklatur für einstrangige Homo- und Copolymere, *Angew. Chem.* **130**(10), 2756 – 2773 (2018) [Translation of IUPAC source-based nomenclature in: *Pure Appl. Chem.* **88**, 1073 – 1100 (2016)].