

Division VIII
Chemical Nomenclature and Structure Representation

Report to IUPAC Bureau, April 2020

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."

The Division Committee met over the period 6–7 July 2019 at the IUPAC GA in Paris, France, with good attendance (20 Committee Members, three Young Observers, one Invited Observer). This was preceded by three-and-a-half days of Task Group meetings (2–5 August), comprising the Alignment, Blue Book, Hydro Prefixes, Inorganic PINs, Metallacycles, Carbon Nanotubes, Graphical Representation and Solid State Terminology project groups. At the Division Committee meeting a decision was made formally to include the Chair of CPCDS as an *ex officio* Division VIII Committee Member, as is already the case with the InChI and JCBN Chairs. The Division Committee also bestowed special recognition and honour on three former members by approving the appointment of Alan McNaught (UK), Warren Powell (USA) and Jeff Leigh (UK) as Emeritus Fellows.

Several new projects have been initiated and approved since the last report, and these are briefly discussed in Section III (below). Of particular note is a new project building on our long-standing liaison with the International Organization for Standardisation (ISO):

'Nomenclature and associated terminology for inorganic nanoscale particles'. This project is co-chaired by IUPAC and ISO representatives and the task group is composed of experts selected by the relevant ISO Technical Committees working in this area and nomenclature experts from Division VIII. The intention is to develop conventions for the clear description of inorganic nanoparticles, their modifications (surface and bulk) and populations, and there is a possibility that the resultant nomenclature may well be InChI-based. This project joins another currently active one on nomenclature for carbon nanotubes and related nanomaterials that is also in collaboration with experts from ISO.

Two other recently approved projects are *'Enhanced recognition and coding of stereoconfiguration by InChI tools'*, which will provide updated procedures allowing InChI to support additional stereochemical cases and avoid mistakes in designation of stereoisomers, and *'Structure-based nomenclature for irregular linear, star, comb and brush polymers with different types of constitutional repeating units (CRUs)'*, which will complement a related and recently concluded project so that polymers containing more than one type of CRU can be easily and uniquely described.

An important current project, *'Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature'*, has 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 recently (February 2020) been published in *PAC*. It is expected that the other projects relying on decisions made in the Alignment project and mentioned in Section III below will now be more rapidly concluded.

Other recent outputs include publication of the *Flavonoids Recommendations* in September 2018, the *Dendrimers Recommendations* in March 2019, the *Lactic Acid-based Polymers Recommendations* at the beginning of 2020, along with the *Guide to Polymer Nomenclature for Authors of Papers and Reports in Polymer Science and Technology (Technical Report)*, and our *Brief Guide to the Nomenclature of Organic Chemistry (Technical Report)*, with the its handy four-page summary brochure as Supplementary Information and available for distribution. Remarkably, translations of the corresponding *Inorganic Brief Guide* (published in 2015) have now appeared in French, Basque, Danish, Dutch, Galician and Spanish, while versions in Catalan, German, Portuguese, Slovak and Thai are in preparation.

Other key priorities are to initiate a new edition of “The Red Book” (*Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005*), possibly in parallel with a new edition of our *Principles of Chemical Nomenclature*, last updated in 2011. We will continue with the revision and further development of the recommendations in “The Blue Book” (*Nomenclature of Organic Chemistry, IUPAC Recommendations and Preferred Names 2013*), and will aim to finalise and publish the several other projects that are nearing completion, as highlighted in Section III (below).

In the last year the Division has made contributions to projects associated with the *International Year of the Periodic Table*, as well as *Building Broader and Deeper Links between OPCW and IUPAC*. The Division continues to support the development of the International Chemical Identifier (InChI) and a successful joint session with the InChI Subcommittee was held at the Paris GA in July 2019. Continued collaboration with the Subcommittee on Polymer Terminology (SPT) of Division IV is ongoing, much valued, and productive in terms of publications related to polymer nomenclature.

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

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), has provided the basis for the completion of several interlinked projects, as several overarching principles have now been established (and further elaborated at the Task Group meetings in Basel in August 2018 and Paris in July 2019). This should now enable rapid progress to be made, and already the boron hydride nomenclature project has been completed and recently published. A priority for this biennium and beyond will be to apply the outcomes of the Alignment Project to complete the projects on metallacycle nomenclature, the Blue Book extension and revision, and preferred names for inorganic compounds (PINs – this means primarily the specification of ligating atoms in coordination compounds, also known as the kappa document). At the Paris meeting in July 2019 it was decided that the latter project should be incorporated into the Alignment project, as kappa problems are similar to those encountered with other modifications of the chemical name (isotopic modifications, etc.). It is anticipated that this will accelerate progress towards the conclusion of these projects.

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, allowing further progress to be made at the Blue Book Task Group meetings in Basel in 2018 and Paris in 2019.

A key project to initiate in this biennium, and which will surely extend into the next few biennia, is to publish a new, updated version of “The Red Book”, *Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005*. 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 concluding project to compile and edit the final book. Discussions in Paris in July 2019 resulted in a first draft of the likely contents and expressions of interest from those likely to take part. The next step is to form a subcommittee to oversee this major undertaking.

The discussions in Paris in July 2019 also identified the need for an updated version of *Principles of Chemical Nomenclature*, last published as the 2nd edition in 2011. As chemical nomenclature becomes broader and more complex, a more accessible and popular exposition of IUPAC recommendations, such as that provided by *Principles*, becomes invaluable in chemistry education and public understanding. Current thinking is that this would run as a project in parallel with a revision of “The Red Book”.

Several long-running projects are nearing completion (these are discussed in Section III, below) and it will be a priority in this biennium to bring these to a conclusion. A complete list of currently active projects can be found in the tabular material at the end of this report (Section IV.2).

The next meeting of the Division VIII Committee, which will be preceded by three days of various associated Task Group Meetings, is currently scheduled for 13 August 2020 at the Ørsted Institute of the University of Copenhagen. In spite of IUPAC financial constraints, it is hoped that a core group of committee members will be able to travel to Copenhagen on the basis of budget available to their Task Groups; while those without funding could join online. At the time of writing, however, it seems that the Covid-19 pandemic might well make travel impossible, in which case we will have to resort to fully virtual Task Group and Committee meetings.

III. Overall report of Division activities and achievements during 2018-2019 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 projects 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. There is no doubt that 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.

In the 2018-2019 biennium several **new projects** were approved and work has started on these:

- *Revision and integration of the carbohydrate related recommendations on Glycoconjugates and Glycoinformatics* (Chair: Vliegthart). 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). The intention of this project was to provide the basis for completion of several projects that were in different states of progress:
 - Boron hydride nomenclature (2012-045-1-800)
 - Metallacycles nomenclature (2013-030-1-800)
 - Preferred names for inorganic compounds, PINs (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; this was reviewed and further work done at a Task Group meeting in Basel in August 2018.

An outcome of task group meetings held before the GA in Paris in July 2019 was the decision to incorporate the PINs (kappa document) project (2006-038-1-800) into the overarching Alignment project (2017-033-1-800) under the new chairmanship of Ture Damhus. The intention is to publish a summary report in *Chemistry International* and then a Recommendation in PAC. Already a successful outcome of the project is that the document on boron hydride nomenclature was able to be finalised and has now been published.

A short summary of the aims of the Alignment project was published in *Chem. Int.* **40**(3), 30 (2018).

- *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. In Paris a draft document was made available.
- *Graphical representation of polymer structures* (Chair: Hellwich). This project had the first task group meeting in June 2018. It 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. Due to the indisposition of Karl-Heinz Hellwich, Andrey Yerin will now chair this task group.

- *Nomenclature and associated terminology for inorganic nanoscale particles* [Co-chairs: Constable (IUPAC)/Brown (ISO)]. This project will begin the development of a framework for the nomenclature of inorganic particles, building upon and refining existing principles derived from polymers, ongoing efforts on carbon nanotubes, ISO terminology, and opportunities with InChI, in addition to developing new frameworks for future materials. The intention is to develop conventions for the clear description of inorganic particles, their modifications (surface and bulk) and populations. The task group comprises members from IUPAC, ISO and relevant technological industries.
- *Enhanced recognition and coding of stereoconfiguration by InChI tools* (Chair: Yerin). InChI tools are widely used as substance identifiers in various sources of chemical information. However, the current support of stereochemical information is limited to tetrahedral, double bond and short allene stereoisomerism. Among the unsupported stereo types are atropisomers and some special cases including centers with more than four ligands. An additional significant problem is an incomplete recognition of configurations for very common Haworth and chair representations of carbohydrates. Updated procedures will allow InChI to support additional stereochemical cases and avoid mistakes in designation of stereoisomers.
- *Structure-based nomenclature for irregular linear, star, comb and brush polymers with different types of constitutional repeating units* (Chair: Chen). This project is intended as a complement to the project ‘Structure-based nomenclature for regular linear, star, comb and brush polymers’ (2013-031-3-800), which provides guidelines for the nomenclature of linear and branched polymers with three or more blocks that are of identical constitutional repeating units (CRUs). This new project will provide guidelines for the nomenclature of the same type of polymers but, importantly, it will extend the nomenclature so that polymers containing more than one type of CRU can be easily and uniquely described.
- **Other new projects** of relevance to Division VIII that were initiated in the 2018-2019 biennium are:
 - * *Chemical and Biochemical Thermodynamics Reunification* (Chair: Iotti).
 - * *Digital Dissemination of Data Standards: Planning for a new Cheminformatics Color Book* (Chair: McEwen).
 - * *IUPAC100 Periodic Table Competition* (Chair: Apotheker).
 - * *International Year of the Periodic Table of Chemical Elements (IYPT) in 2019: planning, coordination and implementation* (Chair: Tarasova).
 - * *InChI Open Education Resource* (Chair: Belford).

- * *Building Broader and Deeper Links Between OPCW and IUPAC* (Chair: Hartshorn/Forman).
- * *Terminology of polymer aggregates* (Chair: Nakano).
- * *Nomenclature of sequence-controlled polymers* (Chair: Théato).

Several projects have been **finalized** or are in the **final stages** of preparation:

- *Nomenclature of flavonoids*. These Recommendations were published in PAC towards the end of 2018.
- *Dendrimers with regular dendrons and hyperbranched polymers*. Recommendations for the nomenclature and terminology of these were published in PAC early in 2019.
- *Boron hydride nomenclature*. As mentioned above, as a result of the Alignment Project meeting in London in November 2017 and follow-up meetings in Basel in August 2018 and Paris in 2019 this document has been finalised, reviewed and was published in PAC early in 2020.
- *Hyphenation of chemical names*. This document, which addresses the needs expressed in discussions with De Gruyter's production department, is now undergoing Division review.
- *Inorganic and Organic Brief Guides*. The *Inorganic Brief Guide* was published in 2015. Its French translation has been prepared with the help of Division VIII and has recently been published (see list of publications in Section IV). Translations are also available in the Basque, Danish, Dutch, Galician and Spanish languages. Versions in Catalan, German, Portuguese, Slovak and Thai are in preparation. The *Organic Brief Guide* was published in PAC early in 2020, and has already been translated into Danish. Both *Guides* were presented as posters at the 'Speed Networking' event at the GA in Paris in 2019.
- *Nomenclature and terminology for linear lactic acid-based polymers* (administered through Division IV) has been finalized, reviewed and was published in PAC early in 2020.
- *A concise guide to polymer nomenclature for authors of papers and reports in polymer science and technology* (administered through Division IV) has been finalized, reviewed and was published in PAC early in 2020.
- A document on *Stereochemical definitions and notations relating to polymers* has undergone Division review, was submitted to ICTNS and is currently nearing the end of its public review period.
- A document on *Nomenclature and terminology for star, comb and brush polymers* has been finalised and is currently under review with ICTNS.
- A document on *Terminology and nomenclature for conjugates based on polymers or other substrates* has been finalized and is currently under review by Divisions IV and VIII.
- A document on *QR codes and industry applications (identifying InChI enhancements)* has been finalized and is currently under Division review.

The outputs of the **six completed projects** for the 2018-2019 biennium mentioned above have been published in PAC and are given full references in the publication listing to be found in the tabular material at the end of this report (Section IV.3).

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). A joint session of the InChI Subcommittee with the Division VIII Committee at the GA in Paris in July 2019 was held, at which the chair of the InChI Subcommittee, Steve Heller, gave an update on the latest developments. The activities of the InChI Subcommittee address 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 now published Organic), we are increasing the value of our efforts in nomenclature by making them available in simplified form to students and authors. Moreover, the value of these outputs is substantially increased by their translation into other languages, for example, the *Inorganic Brief Guide* is now available in French, Basque, Danish, Dutch, Galician and Spanish, while versions in Catalan, German, Portuguese, Slovak and Thai are in preparation.

Revisiting and revising existing IUPAC nomenclature principles and rules as the science of chemistry develops and new classes of compounds 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 was done on several occasions for the Boron Hydride project, and the Lactic Acid Polymers project was presented at a conference in May 2019. Both the Inorganic and Organic Brief Guides were presented at the ‘Speed Networking’ event at the GA in Paris in July 2019.

Our objective of having publishers reproduce the “Brief Guides” in their text books is slowly being realised, and Pearson has recently published the Inorganic Brief Guide as an appendix in the recent 5th edition (2018) of *Inorganic Chemistry* by Housecroft and Sharpe.

Obviously translations of, for example, the *Inorganic Brief Guide*, as highlighted elsewhere in this report, improve both the quality and frequency of communication with stakeholders, and additionally brand IUPAC in the minds of a wider community of stakeholders.

In 2019 Division VIII supported and contributed to the budget of two International Year of the Periodic Table projects which strongly promoted 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 membership list in tabular material at the end of this report, Section IV.1) of 26 elected or appointed members comprises 17 males and 9 females (TMs: 7 male, 3 female; AMs: 4 male, 2 female; NRs: 6 male, 4 female). Our current Vice President is female. There is a reasonable geographical spread, though amongst the TMs and AMs the members are mainly based in Europe or North America. 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.

The recently instituted ‘Emeritus Fellows’ programme can be seen not only as a way of honouring those deserving special recognition, but also retaining their expertise and involvement once no longer eligible for re-election. The Division Committee approved the appointment of three Emeritus Fellows at its meeting in Paris in July 2019: Alan McNaught (UK), Warren Powell (USA) and Jeff Leigh (UK).

Enhance interdivisional interaction and collaboration

Members of Division VIII have been involved in projects administered through the Inorganic Chemistry Division (II), Organic and Biomolecular Chemistry Division (III), and Polymer Division (IV), 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 (SPT), others are involved in projects administered through Division IV, 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. There is also cross-membership with Divisions II and 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 a decision was taken at the Division VIII committee meeting in Paris in July 2019 to include the Chair of CPCDS as an *ex officio* member of the Division VIII committee. One possible initiative is a proposal to develop jointly a Unicode character set for chemistry.

Emphasize multidisciplinary projects addressing critical global issues

Further development of the International Chemical Identifier (InChI) involves multidisciplinary computer scientists and information specialists.

The Division has also been developing closer contacts with organisations which are or will be users of chemical nomenclature. For example, our participation in the IUPAC delegation to the 4th Review Conference of the Organisation for the Prohibition of Chemical Weapons (OPCW) in The Hague in November 2018, with follow-up meetings at the Paris GA in July 2019, is expected to result in a collaborative project with OPCW. This kind of cooperation towards the mutual goal of the peaceful use of chemistry surely epitomizes a project addressing critical global issues.

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. Our new project on inorganic nanoscale particles is now up and running and is jointly chaired as a collaboration between IUPAC and ISO. 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' summarizes the topic in 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, and is also 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. Translations are now

available in French, Basque, Danish, Dutch, Galician and Spanish; versions in Catalan, German, Portuguese, Slovak and Thai are in preparation. More recently, reprints and posters have been prepared for distribution and presentation at relevant conferences or congresses. The publishing house Pearson has included it as an appendix in the recently published 5th edition (2018) of *Inorganic Chemistry* by Housecroft and Sharpe.

The corresponding four-page 'Brief Guide to the Nomenclature of Organic Chemistry' has recently been published (early 2020) and has already been translated into Danish. These Brief Guides should be thought of as quick references and can easily and freely be republished or included in Author Guidelines and textbooks. The 'Polymer Brief Guide' is now due for revision, as a number of new polymer nomenclature documents have appeared since its publication in 2012, and it is intended to initiate this process in the current biennium. There is currently discussion about a similar four-page 'Brief Guide to Biochemical Nomenclature', which would be undertaken in collaboration with JCBN.

Another contribution under the heading of chemistry education is the more popular exposition of IUPAC nomenclature recommendations as provided by the book *Principles of Chemical Nomenclature*, the 2nd edition of which was published in 2011. At the Division Committee meeting in Paris in July 2019 it was decided that a new, updated edition was now desirable, and the way forward for this as a project will be pursued in the current biennium.

Division VIII supported and contributed to the budget of two International Year of the Periodic Table (IYPT) projects in 2019, which will have had obvious impact on chemistry education.

Acknowledgement

The help and advice of Division Secretary Risto Laitinen in the compilation of this report is gratefully acknowledged.

IV. Tabular material

1. DIVISION VIII MEMBERSHIP 2020 – 2021

Name	Status	Term	NAO
Prof. Alan T. Hutton	President	2018-2021	South Africa
Dr. Michelle Rogers	Vice-President	2020-2021	USA
Prof. Risto S. Laitinen	Secretary	2020-2023	Finland
Prof. Michael A. Beckett	TM	2020-2021	United Kingdom
Prof. Edwin Constable	TM	2020-2021	Switzerland
Dr. Karl-Heinz Hellwich	TM	2020-2021	Germany
Dr. Elisabeth Mansfield	TM	2020-2021	USA
Prof. Ebbe Nordlander	TM	2020-2021	Sweden
Prof. Amélia Pilar Rauter	TM	2020-2021	Portugal
Prof. Jiří Vohlídal	TM	2020-2021	Czech Republic
Prof Neil Burford	AM	2020-2021	Canada
Dr. Thomas Engel	AM	2020-2021	Germany
Prof. Robin Macaluso	AM	2020-2021	USA
Dr. Erik Szabo	AM	2020-2021	Slovakia
Prof Augusto Tomé	AM	2020-2021	Portugal
Dr. Clare A. Tovee	AM, <i>CCDC rep.</i>	2020-2021	United Kingdom
Dr. Maria Atanassova Petrova	NR	2020-2021	Bulgaria
Dr. Ture Damhus	NR	2020-2021	Denmark
Prof. Safiye Erdem	NR	2020-2021	Turkey
Mr. Adeyinka Fasakin	NR	2020-2021	Nigeria
Prof. Rafał Kruszyński	NR	2020-2021	Poland
Dr. Ladda Meesuk	NR	2020-2021	Thailand
Prof. József Nagy	NR	2020-2021	Hungary
Prof. Dušan Sladić	NR	2020-2021	Serbia
Ms. Molly Strausbaugh	NR, <i>CAS rep.</i>	2020-2021	USA
Prof. Guoqiang Yang	NR	2020-2021	China
Prof. Richard M. Hartshorn	<i>Ex officio (Sec Gen)</i>	2020-2021	New Zealand
Dr. Steve Heller	<i>Ex officio (InChI)</i>	2020-2021	USA
Leah R. McEwen	<i>Ex officio (CPCDS)</i>	2020-2021	USA
Dr. Gerard P. Moss	<i>Ex officio (JCBN)</i>	2020-2021	United Kingdom
Prof. G. Jeffery Leigh	<i>Emeritus Fellow</i>	2020-2021	United Kingdom
Dr. Alan McNaught	<i>Emeritus Fellow</i>	2020-2021	United Kingdom
Dr. Warren Powell	<i>Emeritus Fellow</i>	2020-2021	USA

2. CURRENTLY ACTIVE DIVISION VIII PROJECTS

Number	Chair	Short Title	Comments
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	to be closed and revived as new project by Rauter
2006-038-1-800	Hartshorn (Damhus)	Inorganic PINs/Kappa Convention	to be merged with 2017-033-1-800 Alignment of principles (Damhus)
2009-022-2-800	Cammack/Ennis (Owen)	JCBN Biologically Important Small Molecules	Owen new Chair - reactivate
2009-040-2-800	Batchelor	InChI Organometallic Compounds	ongoing
2009-041-1-800	Goncharoff	InChI Markush Structures	no feedback
2009-042-1-800	Yerin	InChI Polymers	
2009-043-2-800	Grethe	InChI Reactions	
2011-035-1-800	Jones	Inorganic Polymers (TINCOPS)	Öhrström acting Chair
2011-044-1-300	Brimble	Abbreviations for Protecting Groups	document exists, errata needed
2012-023-2-800	Nicklaus	InChI Tautomerism	document expected
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)	nearly ready for review
2012-039-2-800	Vliegenthart	JCBN Carbohydrate Nomenclature	see 2015-035-2-800 below
2012-046-2-800	Rey (Hartshorn)	InChI Inorganic	transfer to new Chair
2013-010-1-800	Taylor	InChI Biomolecules	possibly close this project
2013-030-1-800	Hutton	Metallacycles	ongoing
2013-031-3-800	Chen	Star Polymers	under review with ICTNS
2013-056-1-800	Mansfield	Carbon Nanotubes	draft document available
2014-001-2-200	Öhrström	Topology of Metal-Organic Frameworks	ongoing
2014-003-2-800	Dijkstra	Hyphenation of Chemical Names	in Division review
2015-003-2-300	Reaney	Homodetic Cyclic Peptides	no feedback – report from Rauter?
2015-019-2-800	Hartshorn	InChI QR-Code Extension	in review
2015-025-4-800	McEwen	InChI Mixtures	ongoing
2015-035-2-800	Vliegenthart	JCBN Carbohydrates [Project extension]	see 2017-026-1-800 below
2015-052-1-800	Hellwich (Moss)	Blue Book Extension and Revision	ongoing (Moss now Chair)
2015-053-1-200	Macaluso	Solid State Terminology	ongoing – draft in progress
2017-026-1-800	Vliegenthart	JCBN Carbohydrates [Project extension]	ongoing
2017-033-1-800	Hellwich (Damhus)	Alignment of Nomenclature Principles	to be merged with 2006-038-1-800 Inorganic PINs (Damhus)
2017-036-2-800	Taylor	Graphic Representation of Reactions	draft document available
2017-039-2-800	Hellwich	Graphic Representation of Polymers	ongoing – Yerin to Chair
2018-005-2-020	Tarasova	IYPT Planning, Coordination, Implementation	
2018-012-3-024	Belford	InChI Open Education Resource	ongoing
2019-016-3-800	Constable/Brown	Inorganic Nanoscale Particles	new project with ISO
2019-017-2-800	Yerin	Stereoconfiguration Using InChI Tools	new
2019-036-1-800	Chen	Star, Comb, etc. Polymers with Different CRUs	new
Also relevant to Division VIII:			
2009-047-1-400	Hellwich (Moad)	Stereochemical Aspects in Polymer Science	under public review
2014-034-2-400	Vert	Polymeric Conjugates	in Division review
2016-046-1-024	Chalk	IUPAC Gold Book Website	ongoing

Continued...

2017-011-3-024 McEwen	Planning Cheminformatics Colour Book	ongoing
2017-021-2-100 Iotti	JCBN Thermodynamics Reunification	ongoing
2019-014-2-400 Nakano	Terminology of Polymer Aggregates	new
2019-041-3-400 Théato	Nomenclature of Sequence-controlled Polymers	new

3. PUBLICATIONS RELATED TO DIVISION VIII SINCE 2018

Recommendations and Technical Reports

A. P. Rauter, M. Ennis, K.-H. Hellwich, B. J. Herold, D. Horton, G. P. Moss, I. Schomburg, Nomenclature of flavonoids (IUPAC Recommendations 2017), *Pure Appl. Chem.* **90**(9), 1429 – 1486 (2018), <https://doi.org/10.1515/pac-2013-091>.

A. Fradet, J. Chen, K.-H. Hellwich, K. Horie, J. Kahovec, W. Mormann, R. F. T. Stepto, J. Vohlidal, E. S. Wilks, Nomenclature and terminology for dendrimers with regular dendrons and for hyperbranched polymers (IUPAC Recommendations 2017), *Pure Appl. Chem.* **91**(3), 523 – 561 (2019), <https://doi.org/10.1515/pac-2016-1217>.

M. Vert, J. Chen, K.-H. Hellwich, P. Hodge, T. Nakano, C. Scholz, S. Slomkowski, J. Vohlidal, Nomenclature and terminology for linear lactic acid-based polymers (IUPAC Recommendations 2019), *Pure Appl. Chem.* **92**(1), 193 – 211 (2020), <https://doi.org/10.1515/pac-2017-1007>.

M. A. Beckett, B. Brellochs, I. T. Chizhevsky, T. Damhus, K.-H. Hellwich, J. D. Kennedy, R. Laitinen, W. H. Powell, D. Rabinovich, C. Viñas, A. Yerin, Nomenclature for boranes and related species (IUPAC Recommendations 2019), *Pure Appl. Chem.* **92**(2), 355 – 381 (2020), <https://doi.org/10.1515/pac-2018-0205>.

K.-H. Hellwich, R. M. Hartshorn, A. Yerin, T. Damhus, A. T. Hutton, Brief guide to the nomenclature of organic chemistry (IUPAC Technical Report), *Pure Appl. Chem.* **92**(3), 527 – 539 (2020), <https://doi.org/10.1515/pac-2019-0104>.

P. Hodge, K.-H. Hellwich, R. C. Hiorns, R. G. Jones, J. Kahovec, C. K. Luscombe, M. D. Purbrick, E. S. Wilks, A concise guide to polymer nomenclature for authors of papers and reports in polymer science and technology (IUPAC Technical Report), *Pure Appl. Chem.* **92**, aop (2020), <https://doi.org/10.1515/pac-2018-0602>.

Other relevant publications

L. McEwen, InChI'ng Forward: Community Engagement in IUPAC's Digital Chemical Identifier, *Chem. Int.* **40**(1), 27 – 30 (2018).

H. Izumi, Consideration of the sequence rule in rule P-94.2, *Chem. Int.* **40**(3), 36 – 37 (2018).

R. M. Hanson, J. Mayfield, M. Vainio, A. Yerin, D. Vladimirovich Redkin, S. Musacchio, Algorithmic Analysis of Cahn-Ingold-Prelog Rules of Stereochemistry: Proposals for Revised Rules and a Guide for Machine Implementation, *J. Chem. Inf. Model.* **58**(9), 1755 – 1765 (2018), DOI: 10.1021/acs.jcim.8b00324.

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)].

Názvosloví anorganické chemie podle IUPAC: Doporučení IUPAC 2005, – česká verze, Jaromír Vinklár, David Sedmidubský (translators), University of Chemistry and Technology, Prague 2018, 380 pp., ISBN 978-80-7080-998-3 [Czech translation of Red Book 2005, with inclusion of new elements].

J. Capitolis, S. Delacroix, X. Frogneux, É. Medina, N. Rey, L. Tinat, S. Carencio, Précis de nomenclature en chimie inorganique, *Actual. Chim.* No. 437, 12 – 17 (2019), [French translation of the Brief Guide to the Nomenclature of Inorganic Chemistry in: *Pure Appl. Chem.* **87**(9-10), 1039 – 1049 (2015)]; <http://www.lactualitechimique.org/Precis-de-nomenclature-en-chimie-inorganique>.

G. J. Leigh, IUPAC and the Periodic Table, *Chem. Int.* **41**(1), 6 – 9 (2019).

E. Scerri, Looking Backwards and Forwards at the Development of the Periodic Table, *Chem. Int.* **41**(1), 16 – 20 (2019).