# **Division** VIII

# Chemical Nomenclature and Structure Representation

# Report to IUPAC Bureau, April 2021

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."

Due to the global Covid-19 pandemic, the Division Committee and associated task group meetings that had been scheduled to be held in Copenhagen during August 2020 had to be cancelled. A virtual Division Committee meeting was held on 19 September 2020, attended by 20 members, and reports were received for all currently active projects and plans made for future Division priorities. Unfortunately the loss of impetus imposed by the absence of physical meetings has hindered the progress of projects within the Division, as members have had to adjust to the new practice of online interactions. It is particularly in the realm of chemical nomenclature, where the minutiae of a recommendation are so important to thrash out, that the light-bulb moments occur in the back-and-forth argument. Hence progress is slower without the face-to-face meetings where the group engages in discussion in front of a whiteboard with a cup of coffee (or beer) in hand.

The Division has been hard-hit by the severe illness (since June 2019) of one of its key members, former President and current TM Karl-Heinz Hellwich, whose encyclopaedic knowledge of chemical nomenclature (and Division VIII institutional knowledge) make him a vital player in Division matters and in many task groups. We continue to wish him and his family strength and hope for a full recovery.

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.

Among 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. Very recently a collaborative project with Division VII has been approved, namely 'A database of chemical structures and identifiers used in the control of WADA prohibited substances'. The Division is currently drafting a proposal to contribute to the CPCDS project on revision of "The Gold Book".

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 *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. This brochure is now also available in a Danish translation. Remarkably, translations of the corresponding *Inorganic Brief Guide* (published in 2015) continue to appear and are now available 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 period under review 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 still to be initiated 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 2<sup>nd</sup> 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 the remainder of 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).

Superimposed on the priorities mentioned above are the participation and commitment required of the Division to contribute to the CPCDS project on '*Development of an IUPAC Recommended Term Management System for Expansion of the Coverage of the IUPAC Compendium on Chemical Terminology*', the so-called 'Gold Book' project. In this the Division will be required to review and, if necessary, update all current entries in the 'Gold Book' relevant to the Division and also scan more recent IUPAC Recommendations for further entries or to revise existing entries. The Division is in the process of developing a project proposal to facilitate this.

The next meeting of the Division VIII Committee, preceded by various associated Task Group Meetings, was scheduled to take place at the 51<sup>st</sup> IUPAC General Assembly in Montreal in August 2021. Regrettably, due to the travel and physical restrictions imposed by the current global Covid-19 pandemic, these meetings will now take place online at the virtual General Assembly platform that is being arranged to replace the physical meeting.

# III. Overall report of Division activities and achievements during the later part of the 2018-2019 biennium and through 2020 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 later part of the 2018-2019 biennium and through 2020 several **new projects** were approved and work has started on these:

- *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, now Damhus). The intention of this project was to provide the basis for completion of several projects that were at different stages, but could not be completed because of their reliance on the conclusions of each other:
  - 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, now Yerin). 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 later part of the 2018-2019 biennium and through 2020 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).
  - \* A database of chemical structures and identifiers used in the control of WADA prohibited substances (Chair: Abbate)

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

- *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, was published in *PAC* early in 2021.
- *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 was

published at the end of 2019 (see list of publications in Section IV.3). 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 tactic polymers* underwent Division, ICTNS and public review and was published in *PAC* towards the end of 2020.
- A document on *Nomenclature and terminology for star, comb and brush polymers* has completed the review processes and is currently in press (*PAC*).
- A document on *Terminology and nomenclature for conjugates based on polymers or other substrates* was reviewed by Divisions IV and VIII and is currently under review with ICTNS.
- A document on *QR codes and industry applications (identifying InChI enhancements)* has been finalized and is currently under review.

The outputs of the **seven completed projects** for the later part of the 2018-2019 biennium and through to early 2021 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). 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 newly 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. The *Organic Brief Guide* has recently been translated into Danish.

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.

Ongoing Division input into the discussions around the report of the Organizational Structure Review Group made available to Bureau towards the end of 2020 will contribute to a new governance structure for IUPAC, an activity which certainly falls under the heading of this subsection of the IUPAC Goals.

#### **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.3 (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 published the *Inorganic Brief Guide* as an appendix in the recent 5<sup>th</sup> edition (2018) of *Inorganic Chemistry* by Housecroft and Sharpe.

Obviously, translations of, for example, the 'Brief Guides', 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 and will become President from 2022. 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 4<sup>th</sup> 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, could 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. 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 *PAC* 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 5<sup>th</sup> 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 *Brief Guide to the Nomenclature of Polymers* 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 2<sup>nd</sup> 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 later part of 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 MEMBERS	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	2020-2021	Finland
Prof. Michael A. Beckett	TM	2020-2023	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, CCDC rep.	2020-2021	United Kingdom
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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, CAS rep.	2020-2021	USA
Prof. Guoqiang Yang	NR	2020-2021	China
Prof. Richard M. Hartshorn	Ex officio (Sec Gen)	2020-2021	New Zealand
Dr. Steve Heller	Ex officio (InChI)	2020-2021	USA
Leah R. McEwen	Ex officio (CPCDS)	2020-2021	USA
Dr. Gerard P. Moss	Ex officio (JCBN)	2020-2021	United Kingdom
Prof. G. Jeffery Leigh	Emeritus Fellow	2020-2021	United Kingdom
Dr. Alan McNaught	Emeritus Fellow	2020-2021	United Kingdom
Dr. Warren Powell	Emeritus Fellow	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	
	) Dixon† (Moss)	JCBN Phosphorus Compounds	to be closed and revived as	
		1 1	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	JCBN Biologically Important Small Molecules	Owen new Chair - reactivate	
	(Owen)			
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		InChI Reactions		
2011-035-1-800		Inorganic Polymers (TINCOPS)	Öhrström acting Chair	
2011-044-1-300	) Brimble	Abbreviations for Protecting Groups	document exists, errata	
			needed	
2012-023-2-800		InChI Tautomerism	document expected	
2012-033-1-800		Graphic Representation of Reactions	see 2017-036-2-800 below	
2012-037-1-800		Hydrogenation (Hydro Prefixes/Indicated H)	nearly ready for review	
2012-039-2-800		JCBN Carbohydrate Nomenclature	see 2015-035-2-800 below	
	) Rey (Hartshorn)	InChI Inorganic	transfer to new Chair	
2013-010-1-800	2	InChI Biomolecules	possibly close this project	
2013-030-1-800		Metallacycles	ongoing	
2013-031-3-800		Star Polymers	in press (PAC)	
2013-056-1-800 2014-001-2-200		Carbon Nanotubes	draft document available	
		Topology of Metal-Organic Frameworks Homodetic Cyclic Peptides	ongoing	
2015-003-2-300	J Keaney	Homodelic Cyclic Peptides	no feedback – report from Rauter?	
2015-019-2-800	) Hartshorn	InChI QR-Code Extension	in review	
2013-019-2-800		InChI Mixtures	ongoing	
2015-025-4-800		JCBN Carbohydrates [Project extension]	see 2017-026-1-800 below	
	) Hellwich (Moss)	Blue Book Extension and Revision	ongoing (Moss now Chair)	
2015-052-1-000		Solid State Terminology	ongoing – draft in progress	
2017-026-1-800		JCBN Carbohydrates [Project extension]	ongoing	
	) Hellwich (Damhus)	Alignment of Nomenclature Principles	to be merged with 2006-038-	
2017 000 1 000	(200000)		1-800 Inorganic PINs	
			(Damhus)	
2017-036-2-800	) Taylor	Graphic Representation of Reactions	draft document available	
2017-039-2-800	•	Graphic Representation of Polymers	ongoing – Yerin to Chair	
2018-012-3-024	4 Belford	InChI Open Education Resource	ongoing	
2019-016-3-800	) Constable/Brown	Inorganic Nanoscale Particles	ongoing project with ISO	
2019-017-2-800	) Yerin	Stereoconfiguration Using InChI Tools	ongoing	
2019-036-1-800	) Chen	Star, Comb, etc. Polymers with Different CRUs	ongoing	
	o Division VIII:			
2014-034-2-400		Polymeric Conjugates	in ICTNS review	
2016-046-1-024		IUPAC Gold Book Website	ongoing	
2017-011-3-024	+ McEwen	Planning Cheminformatics Colour Book	ongoing	

Continued...

2017-021-2-100 Iotti 2019-014-2-400 Nakano 2019-041-3-400 Théato 2020-017-2-700 Abbate JCBN Thermodynamics Reunification Terminology of Polymer Aggregates Nomenclature of Sequence-controlled Polymers Database for WADA Prohibited Substances ongoing ongoing new (9 Nov 2020)

#### 3. PUBLICATIONS RELATED TO DIVISION VIII SINCE LAST GA (PARIS, AUGUST 2019)

#### **Recommendations and Technical Reports**

A. Fradet, J. Chen, K.-H. Hellwich, K. Horie, J. Kahovec, W. Mormann, R. F. T. Stepto, J. Vohlídal, 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), <u>https://doi.org/10.1515/pac-2016-1217</u>.

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.

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#### Other relevant publications

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

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