



Division VIII – Chemical Nomenclature and Structure Representation

Report to IUPAC Council, July 2019

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 13–14 August 2018 in Basel, Switzerland, with good attendance (14 members). This was preceded by three days of Task Group meetings (10–12 August), comprising the Alignment, Blue Book, Hydro Prefixes, Inorganic PINs, Metallacycles, Carbon Nanotubes and Hyphenation project groups.

Several new projects have been initiated and approved since the last report, and these are briefly discussed in Section III (below). In addition to the contribution the Division is making to projects associated with the International Year of the Periodic Table, particularly noteworthy is the new project *Building Broader and Deeper Links Between OPCW and IUPAC*. IUPAC and the OPCW have already signed a Memorandum of Agreement to cooperate towards the mutual goal of the peaceful use of chemistry. Last November IUPAC Divisions and Standing Committees sent representatives to the OPCW Conference in The Hague, and in reciprocation OPCW will send delegates to the upcoming IUPAC GA in Paris in 2019. Division VIII has recently had a follow-up virtual meeting with OPCW officers and it is very likely that a joint project will emerge from these discussions.

Another recent project (*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 recently been finalised and is in the publication phase. 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* last September, the imminent publication of the *Dendrimers Recommendations* (currently in press), and submission for publication of the final version of the *Organic Brief Guide* (in ICTNS review). 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*), 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 to finalise and publish the several other projects that are nearing completion, as highlighted in Section III (below).

Continued collaboration with the International Organisation for Standardisation (ISO) will take place by initiating a project working towards appropriate nomenclature for nanoparticles, and our support for the work of the InChI Subcommittee is ongoing. There are plans for a joint session of the InChI Subcommittee with the Division VIII Committee at the GA in Paris in July 2019.

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 August 2018 Task Group meeting in Basel) that should now enable rapid progress. Already the boron hydride nomenclature project is in the publication phase, and a priority for this biennium and beyond will be to apply the outcomes of the Alignment Project 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.

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 meeting in Basel in August 2018.

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*. 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 in Paris.

We have had a liaison with the International Organisation for Standardisation (ISO) for the past few 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, a project on metal cluster nomenclature will be proposed, 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 next meeting of the Division VIII Committee, which will be preceded by three days of various associated Task Group Meetings, is scheduled for the period 6–7 July 2019 at the IUPAC General Assembly in Paris. There are also plans for a joint session of the InChI Subcommittee with the Division Committee at this meeting.

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), where an asterisk (*) indicates a change in the status or update of the project since the last report. 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. 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.

In the current biennium work has commenced on several **new projects** that have been 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; this was reviewed and further work done at a Task Group meeting in Basel in August 2018. Some details still need to be clarified, which will be done at a Task Group meeting at the GA in Paris. The intention is to publish a summary report in *Chemistry International* and possibly a Recommendation in PAC. Already a successful outcome of the project is that the document on boron hydride nomenclature has been finalised and only needs final polishing for resubmission for publication.

A short summary of the aims of the project has been 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.
- *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.
- *Chemical and Biochemical Thermodynamics Reunification* (Chair: Iotti). This project, originally reviewed by Division VIII and relevant to JCBN, is now fully funded by Division I. It aims at providing a unified approach to the descriptions of the thermodynamics of chemical and biochemical reactions which have historically developed differently in chemistry and biochemistry (approved 14 Nov 2017).
- *Digital Dissemination of Data Standards: Planning for a new Cheminformatics Colour Book* (Chair: McEwen). This short-term project, originally reviewed by Division VIII, is fully funded by the Project Committee and aims at providing the preparative work as basis for the future assembly and production of a Cheminformatics Colour Book (approved 2 Oct 2017).
- *IUPAC100 Periodic Table Competition* (Chair: Apotheker). This project provides the planning and coordination of the online quiz on the Periodic Table conducted during the year 2019 (IYPT and IUPAC 100) (approved 5 Dec 2017).
- *International Year of the Periodic Table of Chemical Elements (IYPT) in 2019: planning, coordination and implementation* (Chair: Tarasova). This project, jointly funded by all Divisions, provides the planning and supports the coordination of events during the IYPT 2019 (approved 26 March 2018).
- *InChI Open Education Resource* (Chair: Belford). This project aims at providing an online platform with educational material about InChI as well as a discussion forum on this material (approved 28 Feb. 2019).
- *Building Broader and Deeper Links Between OPCW and IUPAC* (Chair: Hartshorn/Forman). IUPAC and the OPCW have signed a Memorandum of Agreement to cooperate towards the mutual goal of the peaceful use of chemistry. In this project, IUPAC Divisions and Standing Committees sent representatives to the OPCW Conference in The Hague last November, and in reciprocation OPCW will send delegates to the upcoming IUPAC GA in Paris in 2019. Follow-up virtual

meetings will result in a report for *Chemistry International* and possible joint projects going forward.

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 and follow-up meeting in Basel in August 2018 this document has been finalised and only needs some minor polishing before resubmission to PAC.
- *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. 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* is currently in ICTNS review.
- *Nomenclature and terminology for lactic acid-based polymers* (administered through Division IV) is currently in public review.
- *A concise guide to polymer nomenclature for authors of papers and reports in polymer science and technology* (administered through Division IV) is close to resubmission for publication.
- A document on *Stereochemical definitions and notations relating to polymers* has undergone Division review and is close to submission to ICTNS.
- A document on *Nomenclature and Terminology for Star, Comb and Brush Polymers* is currently undergoing finalisation for submission to ICTNS.

Thus far the following projects have been **completed** during the current biennium:

- *Nomenclature of Flavonoids* (IUPAC Recommendations 2017), *Pure Appl. Chem.* **90**(9), 1429 – 1486 (2018), DOI: 10.1515/pac-2013-0919.
- *Nomenclature and terminology for dendrimers with regular dendrons and for hyperbranched polymers* (IUPAC Recommendations 2017), *Pure Appl. Chem.* **91**(3), 523 – 561 (2019), DOI: 10.1515/pac-2016-1217.

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). There are plans for a joint session of the InChI Subcommittee with the Division VIII Committee at the GA in Paris in July 2019. 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 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 has been done recently for both the Inorganic Brief Guide and Boron Hydride projects, and the Lactic Acid Polymers project will be presented at a conference in May 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.

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 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 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 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 in The Hague last November has recently resulted in a request for a collaborative project from OPCW leadership. 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. 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 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. Reprints and posters have also 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.

A similar four-page Brief Guide to the Nomenclature of Organic Chemistry has been submitted for ICTNS review. These Brief Guides should be thought of as quick references, and can easily 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.

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 (*status change since last report)

Number	Chair	Short Title	Comments
*2001-081-1-800 (Kahovec)	Fradet	Nomenclature for Dendrimers	published March 2019
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	published Sept. 2018
*2009-022-2-800 (Cammack/Ennis)	Owen	JCBN biologically important Small Molecules	reactivate
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	
*2009-047-1-400	Hellwich	Stereo Poly	imminent submit to ICTNS
*2010-055-1-800	Hartshorn	Inorganic and Organic Brief Guides	part 1 published, part 2 ICTNS
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)	finalise for review
2012-039-2-800	Vliegenthart	JCBN Carbohydrate Nomenclature	see 2015-035-2-800 below
*2012-045-1-800	Beckett	Boron Nomenclature	resubmit for publication
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	finalise for review
*2015-003-2-300	Reaney	Homodetic Cyclic Peptides	no feedback
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	ongoing
2015-053-1-200	Macaluso	Solid State Terminology	
2017-026-1-800	Vliegenthart	JCBN Carbohydrates [Project extension]	
*2017-031-1-050	Apotheker	IUPAC 100 Periodic Table Competition	
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	
*2018-005-2-020	Tarasova	IYPT Planning, Coordination, Implementation	
*2018-012-3-024	Belford	InChI Open Education Resource	
*2018-022-3-020	Hartshorn/Forman	Building links between OPCW and IUPAC	
Also relevant to Division VIII:			
2006-004-1-400	He	Abbreviations for Polymer Names	completed, errata needed
*2008-020-1-400	Hodge	Web Guide to Polymer Naming	resubmit
*2014-033-1-400	Vert	Lactic Acid Polymers [Project extension]	in public review
*2017-011-3-024	McEwen	Planning Cheminformatics Colour Book	
*2017-021-2-100	Iotti	JCBN Thermodynamics Reunification	

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

(** = added since last report, April 2018)

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).

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. 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), <https://doi.org/10.1515/pac-2016-1217>.

Other relevant 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).

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

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).

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>.