International Union of Pure and Applied Chemistry
Division VIII
Chemical Nomenclature and Structure Representation

Minutes of Division Committee Meeting
Paris, France, 6–7 July, 2019

1. Welcome, introductory remarks and housekeeping announcements

Alan Hutton (ATH) welcomed everybody to the meeting, extending a special welcome to those who were attending the Division Committee (DC) meeting for the first time. He described the house rules and arrangements for the meeting.

2. Attendance and apologies

Present for all or part(s) of the meeting: Alan T. Hutton (President, ATH), Risto S. Laitinen (Secretary, RSL), Michael A. Beckett (MAB), Neil Burford (NB), Ture Damhus (TD), Richard M. Hartshorn (RMH), Steve Heller (SH), Robin Macaluso (RM), Elisabeth Mansfield (EM), Ladda Meesuk (LM), Gerry P. Moss (GPM), Ebbe Nordlander (EN), Maria A. Petrova (MAP), Amelia P. Rauter (APR), Michelle M. Rogers (MMR), Molly A. Strausbaugh (MAS), Erik Szabó (ES), Clare Tovee (CT), Jiří Vohlídal (JV), Andrey Yerin (AY)

(For the Division VIII membership in 2018-2019 and the group photo of the participants, see Appendix 1)

Invited observer: G. Jeffery Leigh (GJL)

Young observers: Christine E. Dunne, Lori Ferrins, Matteo Lusi

Apologies: Fabio Aricò (FA), Edwin C. Constable (ECC), Ana Maria da Costa Ferreira (ACF), Karl-Heinz Hellwich (Past-President, KHH), Rafał Kruszyński (RK), Keith T. Taylor (KTT)

Visit by IUPAC officers: Qi-Feng Zhou (President of IUPAC), Christopher M.A. Brett (Vice-President of IUPAC), Richard M. Hartshorn (Secretary-General of IUPAC)

No replies: Sangho Koo, Safiye Erdem, József Nagy

3. Introduction of attendees

A short round of introductions was made. Maria Petrova (MAP), Ladda Meesuk (LM, who was present only in the cross-over meeting of Divisions II and VIII) and Erik Szabó (ES) were attending the meeting of the Division Committee for the first time.

ATH reported that the Past-President of Div. VIII, Karl-Heinz Hellwich, who had been nominated as a Titular Member for the 2020-2021 biennium, is seriously ill. His recovery is expected to take a long time. ATH noted that in addition to the personal tragedy, the loss of KHH is very serious for the Division.

4. Approval of agenda

The agenda was approved (see Appendix 2), though it was noted that the order of discussion of various agenda items may need to be adjusted due to conflicts in the schedule.

5. Approval of minutes of meeting in Basel, 13–14 August 2018

The discussion of and decision on this item were postponed to the end of the current meeting, when some modifications that had been suggested for the draft minutes of the Basel meeting were adopted. At the end of the meeting, the minutes were approved as modified.

There was also a brief discussion about the level of detail in the minutes. TD noted that detailed minuting is important for understanding the reasons and justification behind any decisions made.

6. Matters arising

It was concluded that all matters arising will be discussed in connection with other items on the agenda.

7. Division Rules

The draft Division Rules (Appendix 3) had been circulated and some comments were received. There were several points that came up in the discussion:

TD noted that the document was symptomatic of too much bureaucracy. He also objected to the strict rules for expulsion of members who might not have been active for two or more years. As everyone was working as a volunteer, the time frame was too tight. RSL noted also that the restrictions for the time of service in the Division were too short. The development of nomenclature was slow and required general agreement of the scientific community. It was more important to produce good rather than fast recommendations. GPM agreed and remarked that it took several years before people were confident enough to write documents. AY noted that no sooner had people accumulated experience, than they were obliged to retire.

EN asked why the rules were being put forward for acceptance by the Council at the GA in Paris, when everybody was in agreement that there were aspects that were unacceptable. ATH agreed with this sentiment, but noted that the Divisions were given very tight time constraints to draft the rules, which were largely based on those of Division I. The rules had to be submitted to the IUPAC Secretariat by March, and the comments were received only afterwards. He explained that these rules could always be modified to suit the particular requirements of Division VIII, when the need arose.

TD wanted it to be mentioned in the minutes that he objected to this kind of handling of the Division Rules. EN seconded this sentiment, and everybody was in agreement.

The Committee agreed that the Chairs of the Division VIII Subcommittees should be *ex officio* Members of the Division Committee (see also Item 13.1).

8. Division VIII Emeritus Fellows Program

The new Division VIII Emeritus Fellows Program was endorsed. It is stated in the Division Rules that "This category of membership will be bestowed upon meritorious individuals who have *earned by service* a special recognition *upon their retirement* (departure) from one or more Division VIII administrative posts or from a multiple of key Division VIII Project roles." It was thought more appropriate that Emeritus Fellows be appointed from scientists who were no longer eligible for re-election, rather than on their retirement. This would be a mechanism to keep people involved. It was also decided that Emeritus Fellows need to have been members of Division VIII. A list of Emeritus Fellows may be found on the IUPAC website.

The Division Committee nominated and elected the first three Emeritus Fellows of Division VIII: Warren Powell, Alan McNaught and Jeff Leigh.

9. Interactions between Division VIII and other (IUPAC) bodies in relation to documents and projects involving chemical nomenclature.

Division I. The Division VIII contact person is Risto Laitinen (the Division I counterpart is Roberto Marquardt). RSL reported that there had been no contact during the past year.

Division II. The contact person is Robin Macaluso, who is also a TM in Division II during the 2018-2019 biennium (the formal Division II counterpart is Daniel Rabinovich).

Division III. The contact person is Amélia Rauter, who is also the Secretary of Division III (and thus serves as the Division III counterpart).

Division IV. The contact person is Jiří Vohlidal (the Division IV counterpart still unclear). Both KHH and JV are members of SPT, providing natural overlap. The overlap with SPT is so important that it would be good to have two contact persons. It was decided that Andrey Yerin continues to be a co-contact.

Division V. Risto Laitinen is the contact person for Division V (with M. Clara Magalhães as the Division V counterpart).

Division VI. Edwin Constable will be contact person for Division VI (the Division VI counterpart is yet to be established).

Division VII. Ture Damhus is contact person for Division VII (with Helle Møller Johannessen as the Division VII counterpart).

> ***Action:*** The reactivation of contact relationships will be continued. RSL will interact with the Secretaries of those Divisions which do not yet have a contact person.

ICTNS. Ture Damhus is the representative of Division VIII on ICTNS. TD reported that ICTNS had now acknowledged that there were problems with the handling of the review process and corrective actions were being taken.

InChI Subcommittee. Andrey Yerin (AY) continues as the Division VIII representative on the InChI Subcommittee. It was agreed that contact with the InChI Subcommittee needs to be expanded, since much of their work is directly related to Division VIII interests (see also Item 10.4).

SPT (Subcommittee on Polymer Terminology) had formulated instructions on how the submission process for completed projects should work. JV is the Division VIII representative in SPT.

CPCDS (Committee on Printed and Cheminformatics Data Standards). CPCDS is a Standing Committee of IUPAC. AY is a member of the Subcommittee on Cheminformatics Data Standards (SCDS), as well as a member of the InChI Subcommittee, which is a Division VIII subcommittee.

CPCDS had expressed interest in closer contacts with Division VIII. The contacts with the InChI Subcommittee also needed to be intensified.

> ***Action:*** (i) CPCDS to be contacted to nominate a representative to join the Division VIII roster. (ii) Clare Tovee to be proposed as a second Division VIII representative on the InChI subcommittee.

ISO (International Organization for Standardization). While there is currently no official Division VIII representative, ECC was willing to represent Division VIII. Communication with ISO was important, for instance, in connection with nanoparticles and carbon nanotubes.

CCDC (Cambridge Crystallographic Data Centre). CCDC had nominated Clare Tovee as an AM to the Division VIII Committee. She is thus the natural contact between the two organizations.

Wikipedia. There was extensive discussion about the problems involved in the handling of nomenclature in Wikipedia. Anybody could make modifications to Wikipedia articles, but often the work of specialists was ignored. Therefore, there was the possibility for wrong or inaccurate nomenclature being presented. Thus far, no satisfactory solution had been found to this problem and it was thought that, at least for the present time, no task group or subcommittee needed to be established. RMH suggested that those items that should not be modified by anybody should be incorporated as images rather than text.

JCBN (Joint Commission on Biochemical Nomenclature). GPM is the chairman of JCBN, TD and APR are Associate Members, and ATH is a member *ex officio*. JCBN is a Joint Commission of IUBMB and IUPAC. GPM noted that while IUPAC dealt with chemical nomenclature, IUBMB dealt with enzyme nomenclature. There is a glossary providing IUPAC equivalents to the biochemical names that abound in the enzyme database. A significant contribution was coming from IUPAC. Enzyme entries were constantly updated and augmented or deleted. TD noted that JCBN had a very relaxed way of handling memberships regardless of their origin.

REACH (Registration, Evaluation, Authorization and Restriction of Chemicals). MMR reported that after the scoping exercise it was now time to set up a project. As companies generally provided

names which do not conform with IUPAC names, the successful outcome of the project would depend on the interest shown in adopting IUPAC names.

> ***Action:*** A formal task group (MMR, TD, MAS) will be formed. Its brief would be to see if there was sufficient interest from the chemical industry. The contact with CEFIC (European Chemical Industry Council) could be useful.

ACS Nomenclature Committee. MMR and MAS are the contact persons. In 2019 the Committee on Nomenclature, Terminology and Symbols (NTS) project teams started to make significant progress in working towards the Vision and Mission of the committee. Below are some of the key accomplishments of each of the project teams related to their particular goals:

Goal 1: Achieve a common language of chemistry by educating its practitioners. The project team is in the process of developing a training workshop for K-16 educators on the teaching of chemical nomenclature. They hope to present the workshop at the Biennial Conference on Chemical Education (BCCE) 2020. Based on the development work for this workshop they plan on extending the reach through an American Association of Chemistry Teachers (AACT) webinar.

Goal 2: Facilitate the interaction of chemists to implement appropriate chemical representations. NTS and CNIF co-organized a day-and-a-half symposium in San Diego entitled: "Chemical Nomenclature and Representation: Past, Present and Future". The symposium examined the importance of having a common language for chemistry from the inception of IUPAC 100 years ago to the need for chemical representation that can be read by both humans and computers today.

NTS submitted comments on two IUPAC Recommendations: "Recommendations and terminology for lactic acid-based polymers" and "Definition of the chalcogen bond".

Goal 3: Advocate for the use of a common language of chemistry. NTS supported an update of the ACS Style Guide by reviewing and proposing updates to the sections focused on chemical nomenclature, terminology and symbols. A review of NTS stakeholders was conducted and resulted in the creation of a stakeholder chart supporting their internal and external engagement, collaboration, education and advocacy efforts.

NTS, in collaboration with the Braille Authority of North America, has facilitated discussions with visually impaired chemists to standardize the Braille code for chemistry. Through this collaboration, NTS is jointly working to improve the ability of the code to represent chemical structures, increase the usage of the code through advocacy and outreach, and remove redundancy in the existing code. Discussions have been held with Braille transcribers and the project is on track for targeted completion by the end of 2019.

CAS. The Chemical Abstracts Service is an important interactive body for Division VIII. MAS is the liaison there (current AM, later NR, and a CAS representative).

RSC. GPM is the Chair of the RSC Committee on Standards in Nomenclature, Terminology, Units and Symbols and is the contact person for Division VIII. During the last meeting of the committee, it was expressed that IUPAC needs a better system to distribute documents for public review, since RSC would like to review every document.

10. Reports on Division VIII projects

10.1. Building broader and deeper links between OPCW and IUPAC (proposal 2018-022-2, Richard Hartshorn)

RMH noted that there was a report on the interaction between IUPAC and OPCW in the April issue of *CI*. The objective was to widen the interaction between OPCW and IUPAC and to increase mutual understanding of the work of both bodies in order to establish what cooperation might be established. The Division representative is ECC. A significant problem was that the people in OPCW are term-limited to seven years. There are people interested in nomenclature, but their terms are finishing at the end of 2019. It was hoped that Division VIII would establish projects with OPCW. The goal was to get OPCW representatives to come to the GA in Paris, but this did not work out due to schedule conflicts.

10.2. Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature (2017-033-1-800, Karl-Heinz Hellwich)

TD reported on the Task Group meeting, which took place in Paris just prior to the Division Committee meeting. The consensus in the Task Group was that the project *Preferred names for inorganic compounds (2006-038-1-800)*, which was popularly called '*Inorganic PINs'* (see Item 10.17), should be incorporated in the present *Alignment Project* to include development of the kappa notation, since the problems around kappa were similar to those of other modifications of the name (isotopic modifications, etc.). The ordering of the various modifications was decided in London in 2017. The problem was that the inclusion of kappa in a name could change the whole name. This work needs to continue. The second part of the '*Inorganic PINs'* project involved the central atoms. That was a separate issue, but it should be easier to handle. The *Metallacycles Project* (see Item 10.9), on the other hand, should remain as an independent project which, however, monitors closely the results of the *Alignment Project*.

TD will take over as Chair due to the indisposition of KHH. The project will deal with the further developments of kappa nomenclature already discussed for some years now and the alignment of the specification of coordinating atoms with other descriptors, particularly isotopic modification descriptors, stereodescriptors and the specification of non-standard bonding numbers. Later on, the sub-project about selecting and ordering central atoms will be taken up again.

At the Task Group meeting it had been agreed that TD should work at an exposition wherein the most general name for a complicated ligand was a fully substitutive name, with all substituent groups having different modifiers being cited separately. (A preliminary document of this kind already existed and was circulated in November 2017. A major change to be made to it was to ensure that there was always only one substituent group cited as a suffix, as strongly advocated by the Task Group.)

The relative ordering of modifiers becomes important, for example, when certain suffixes upon modification have to be changed to prefixes; the choices will be based on decisions made at the London 2017 meeting, as summarized in Appendix 3 of the Basel 2018 Division VIII minutes.

Simplification will thereafter be possible in a number of cases, so that well-known names such as presented in the *2005 Red Book* will hopefully drop out as equally acceptable alternatives to the elaborate general names. In particular, multiplicative names will not be admitted in the general case where symmetry is broken, but should be possible in simple cases, *e.g.*, when the parents being multiplied are modified identically or the modification for other reasons can be specified unambiguously outside the name itself.

The idea of using a canonical numbering for the specification of sites of modification was discussed at the Task Group meeting and had been rejected.

The *Metallacycles Project* (2013-030-1-800, see Item 10.9) will continue as a separate project. It does not fundamentally depend on the developments of kappa nomenclature yet to be worked out in the *Alignment Project*.

> ***Action:** (i) The *Alignment Project* and the *Inorganic PINs Project* will be merged together (see Item 10.17). (ii) The Task Group will consist of members of the original Task Groups, namely: Ture Damhus (Chair), Michael A. Beckett, Edwin C. Constable, Richard M. Hartshorn, Karl-Heinz Hellwich, Alan T. Hutton, Risto S. Laitinen, Gerard P. Moss, Ebbe Nordlander, Warren Powell and Andrey Yerin. (iii) The agreed time plan: before 1 October 2019, TD will send out a number of examples, both simpler and more complicated ones, to be considered as the basis for formulating rules, and the Task Group members should respond with their suggestions and comments before 1 December 2019.

10.3. Graphical representation standards for chemical reaction diagrams (2003-045-3-800/2012-033-1-800/2017-036-2-800, Keith T. Taylor)

In the Task Group meeting in Paris prior to the Division Committee meeting, KTT reported on a draft document and had received comments from those present. Progress was made, but the document was not yet ready for publication. The last part of the document involved mainly practices for publishers and these aspects were therefore not commented on in the Task Group meeting.

10.4. IUPAC International Chemical Identifier (InChI) projects

Steve Heller (SH) attended this part of the meeting. As a subcommittee Chair he is *ex officio* a member of the Division VIII Committee. In addition to his oral report during the meeting on current aspects concerning the InChI Subcommittee, he provided a formal written report (see Appendix 4).

The InChI Subcommittee was satisfied with their terms of reference, which are shown as an appendix to the Division VIII Rules (see Appendix 3). SH noted that InChI was the first, and thus far only, example of IUPAC going digital. It had been agreed in 2000 that the InChI standard would become the standard for IUPAC. This has been a success story in case of organic compounds, but there are problems with inorganic species. He noted that the activities of the subcommittee are focused on the development of the algorithm and are not concerned with search methods.

SH also reported on the current status of the following projects:

10.4.1. InChI extension for mixture composition (2015-025-4-800, Leah McEwen)

The project is and will remain operational.

10.4.2. Identifying International Chemical Identifier (InChI) enhancements – QR codes and industry applications (2015-019-2-800, Richard Hartshorn)

The standard for the QR codes could be finalized by the end of September. Then the software needs to be written – this will be done by Jeremy Frey.

10.4.3. Implementation of InChI for chemically modified large biomolecules (2013-010-1-800, Keith Taylor)

This project has not progressed far and will be closed.

10.4.4. Handling of inorganic compounds for InChI V2 (2012-046-2-800, Richard Hartshorn and Hinnerk Rey)

HR has not been active for three years but has now resurfaced and has agreed that he can continue the work. TD stated that he can provide information about inorganic chemistry, but organometallic compounds are rather problematic.

10.4.5. Redesign of handling of tautomerism for InChI V2 (2012-023-2-800, Marc Nicklaus)

There were 60–70 examples that have now been worked to completion. A document could be expected within the next few months.

10.4.6. InChI requirements for representation of organometallic and coordination compound structures (2009-040-2-800, Colin Batchelor)

The contract has been signed to develop the algorithm for organometallic and coordination compounds. Initial results will be discussed in San Diego during the ACS National Meeting. The important thing is that the software should work. InChI is an algorithm, and the aim of the algorithm is to provide a good, reliable representation.

10.4.7. InChI Open Education Resource (OER) (2018-012-3-024, Robert Belford)

This education project is progressing nicely. A poster will be presented in Paris and the website is functional. The main problem is that chemistry institutions are not yet aware of InChI. There is a YouTube video publicizing and explaining InChI which may be found at the following URL: https://www.youtube.com/watch?v=rAnJ5toz26c .

10.5. Corrections, revisions and extension for the nomenclature of organic chemistry – IUPAC Recommendations and Preferred Names 2013 (the IUPAC Blue Book) (2015-052-1-800, Karl-Heinz Hellwich)

Due to the indisposition of KHH, GPM will take over the project. There were a number of things in Basel that needed action (for example, stereochemistry). After Basel, stereochemical and other corrections had been made. A large number of corrections was processed according to page

numbers, themes, *etc*. A batch of *ca*. 50 corrections was put on the Internet every week (*ca*. 3000 overall). GPM was now in the act of producing a HTML version of the entire Blue Book incorporating all the corrections.

10.6. Nomenclature of carbon nanotubes and related substances (2013-056-1-800, Elisabeth Mansfield)

EM reported that the work was currently concerned with modifying the chiral index (now called the structure index). The Task Group met in Paris and had made good progress. The document was in a well-advanced stage. There will be a Recommendation soon, which will grow out of the existing report.

10.7. End-of-line hyphenation of systematic chemical names (2014-003-2-800, Albert Dijkstra)

After KHH became ill, Jan Reedijk finalized the draft for comments. ES had made substantial suggestions for modifications. There was now a new version, so the previous one should not be reviewed.

***Action:** ATH will send a new version for commenting, when available.

10.8. Terminology guidelines and database issues for topology representations in coordination networks, metal-organic frameworks and other crystalline materials (2014-001-2-200, Lars Öhrström)

This is a Division II project in which Division VIII has an active interest. It was decided in Paris during the crossover meeting between Divisions II and VIII (see Item 15.2.1) that Neil Burford should be the liaison for Division VIII in this project.

10.9. Nomenclature for metallacycles containing transition metals (2013-030-1-800, Alan Hutton)

ATH reported that during the meeting of the Task Group in Paris, the main discussion was concerned about the naming of charged metallacycles.

***Action:** ATH will prepare a new version of Sections 1–3 of the document, TD will prepare the new version of Section 4 about charged metallacycles and RSL will prepare any figures.

10.10. Nomenclature for polyhedral boranes and related compounds (2012-045-1-800, Michael Beckett)

MAB reported that finally progress had been made and the manuscript had been submitted to PAC in May. He was informed during the meeting that the document has been accepted for publication.

10.11. Revision and extension of IUPAC recommendations on carbohydrate nomenclature (2012-039-2-800, 2015-035-2-800, 2017-026-1-800 Johannes Vliegenthart)

APR reported that the Task Group had a very fruitful meeting in Braunschweig. The document was almost finished. Only the glycolipids still needed to be considered. There were two goals for the project: revision of the document and the integration of carbohydrate conjugates. This task had turned out to be more extensive than was originally anticipated. A second extension of the project was applied for and had been approved. A considerable part of the nomenclature section was revised at a meeting in Cambridge in the spring of 2018. TD noted that glycoinformatics researchers were discussing how to define a carbohydrate. There was a need to increase the interaction between synthetic chemists and those involved with informatics. GPM said that there had been a long discussion about this project in ICTNS. The next stage would be the submission of the document to ATH for distribution to the whole Division roster.

10.12. A comparison of assignment of hydro prefixes, added and indicated hydrogens in IUPAC, CAS and Beilstein nomenclature systems (2012-037-1-800, Andrey Yerin)

AY reported that TD and AY had reviewed the document in Paris. It was almost complete but still needed several clarifications. Some corrections were needed and a few references were missing. Additional examples would also improve the manuscript.

10.13. Terminology and nomenclature of inorganic and coordination polymers (also known as 'TINCOPS', 2011-035-1-800, Richard Jones)

TD reported that there had been no progress over the last year. The aim of the project was to update an old IUPAC Recommendation from 1984 [*Pure & Appl. Chem.* **57** # 1 (1985) 149-168]. It was worth noting that the old document had been reprinted, unchanged, in the *2000 Red Book* (Chapter II-7). New drawings needed to be made, and the kappa convention needed to be taken into account.

10.14. Brief guides to the nomenclature of organic and inorganic chemistry (so-called 'Essentials' of organic and inorganic nomenclature) (2010-055-1-800, Richard Hartshorn and Karl-Heinz Hellwich)

RMH informed the Division Committee that since KHH was not able to submit the files of the *Organic Brief Guide*, RMH had submitted the document for ICTNS and public review. There had been several referees involved, with some still to respond. GJL noted the importance of checking for consistency between the Red (Inorganic), Blue (Organic) and Purple (Polymer) Guides.

10.15. Glossary of small molecules of biological interest (2009-022-2-800, Gareth Owen)

The original objective was to provide nomenclature rules for molecules of biological interest that were not covered in other documents due to the lack of suitable compound classes. There was a need for a simple document dealing only with some important small molecules of biological interest, rather than for the production of the full-scale database. The current Chair of the Task Group is Gareth Owen.

10.16. Nomenclature of flavonoids (2009-018-2-800, Amelia Rauter)

The final manuscript was published in *PAC* in 2018 (see Appendix 6) and this project is complete.

10.17. Preferred names for inorganic compounds (2006-038-1-800, Ture Damhus)

This project, popularly known as '*Inorganic PINs'*, should be closed. TD had proposed this at the Task Group meeting, and RMH supported abandoning the concept of inorganic PINs based on his consultations with the European Union's customs authorities just before the Paris meetings.

The themes dealing with the kappa convention and the central atoms will be merged with the *Alignment Project* (see details under Item 10.2).

10.18. Nomenclature of phosphorus-containing compounds of biochemical importance (2006-019-1-800, Gerard Moss)

This project will be closed. There will a new project with APR as a chair.

10.19. Polymer projects (with Division IV)

During the crossover meeting between the Divisions IV and VIII, Roger Hiorns reported on the status of the polymer projects (see Item 15.2.2).

10.19.1. Graphical representation of polymer structures (2017-039-2-800, Karl-Heinz Hellwich)

This project started last year and was proceeding well. AY will be the coordinator for Division VIII. Patrick Théato will coordinate from Division IV. In time a representative from Division VIII will be needed.

10.19.2. Nomenclature for polymeric carriers bearing chemical entities with specific activities and names (2014-034-2-400, Michel Vert)

The project is near to completion.

10.19.3. Structure-based nomenclature for regular linear, star, comb and brush polymers (2013-031-3-800, Jiazhong Chen)

The project is near to completion. Jiazhong Chen is planning a follow-up project.

10.19.4. Definitions and notations relating to stereochemical aspects in polymer science (2009-047-1-400, Karl-Heinz Hellwich and Graeme Moad)

The document has been submitted to ICTNS.

10.19.5. Revision of IUPAC Recommendations on macromolecular nomenclature – Guide for authors of papers and reports in polymer science and technology (2008-020-1-400, Philip Hodge) (Web-based IUPAC recommendations on polymer nomenclature)

The document has been submitted to *PAC*.

10.19.6. Preferred names for polymers – a list of preferred, acceptable (other IUPAC-approved) and not acceptable (ambiguous, wrong or outdated) names for polymers (2008-015-1-400)

Published.

10.19.7. Guidelines for abbreviating polymer names (2006-004-1-400)

Published.

10.19.8. Terminology and structure-based nomenclature of dendritic and hyperbranched polymers (2001-081-1-800, Alain Fradet and Jaroslav Kahovec)

Published.

10.20. Survey of definitions and use of common solid-state chemistry terminology (2015-053-1-200, Robin Macaluso)

RM reported that a Technical Report was currently being written on the findings related to solid-state terminology. The Task Group had decided to focus the report on crystalline solids, as defined by the International Union of Crystallography. Crystalline materials would be discussed in the report with respect to bonding and the bonding tetrahedron (with each corner defined as ionic, covalent, van der Waals, metallic). The bonding tetrahedron itself was not a new concept, but it has not been explicitly discussed in light of crystalline solids.

The concept of liquid crystals would also be discussed and this was expected to lead to a future project. In addition to the report, the Task Group would pursue an educational component of the project. Conversations would be initiated with the creator of CrystalMaker software to produce crystal structure images that would help to explain bonding in crystalline solids.

The Task Group would continue working on the structured draft in Paris during their meeting following the Division Committee meeting. It was anticipated that a report could be submitted for review within six to nine months. There had been some delay in the progress of the project due to the Chair taking maternity leave.

During the discussion, TD noted that this project was a good example of combining terminology with nomenclature. JV enquired whether this project was about inorganic materials to which RM replied with an affirmative. Only inorganic crystalline materials were being considered and that excluded species like polymers. Parts of this project could be incorporated in the *Red Book* revision.

10.21. Nomenclature of homodetic cyclic peptides produced from ribosomal precursors (2015-003-2-300, Martin Reaney)

No information [project terminated 2 December 2019].

10.22. IUPAC color book data management (2013-052-1-024, Kinnan)
[Note: This project has been closed and repurposed as *Backup, maintenance and redevelopment of the IUPAC Gold Book website (2016-046-1-024, Stuart Chalk)*]

GPM reported on the presentation (given to ICTNS) by the current Task Group Chair, Stuart J. Chalk, on the vision for the development of the *Gold Book*. There will be a new design, which would be suitable for computer, tablet and mobile platforms. New features would include REST URLs, API

and Global Search. Data would be stored in a database and will be easy to update and manage. The website will be backed-up and maintained using GitHub (see https://github.com/iupac).

The project is divided into three phases: (1) development of an IUPAC Recommended Terms Management System (RTMS); (2) curation of IUPAC Recommended Terms into a Term Management System; and (3) development of an IUPAC Chemical Ontology (to be started after the completion of phases (1) and (2).

During the next couple of years the Divisions would be requested to look at each relevant entry in the database to see whether they were correct or if something was missing or erroneous (see also Item 15.3).

10.23. Rules for abbreviating protecting groups (2011-044-1-300, Margaret Brimble)

APR reported that the project still had money and that the work continued. There was an existing document, but there were names that need to be revised according to the current *Blue Book* rules. This would be handled by creating a list of errata.

11. Future projects/activities

11.1. International Organization for Standardization (ISO) liaison. Nanoparticles projects

ATH reported that there would be two projects in the domain of nanoparticles. There was already an established project working on the nomenclature of carbon nanotubes (see Item 10.6). ECC and Stuart Brown (from ISO) were preparing a project proposal for the nomenclature of clusters. The Task Group comprised ECC, RMH, MAB and AY from Division VIII, and Stuart Brown and several other people from ISO.

11.2. New edition of Nomenclature of Inorganic Chemistry, the 'Red Book'

ATH and RMH suggested that the *Red Book* revision should consist of a number of small projects, some of which were already active. The Division Committee could be overseeing the work. There could be a scoping project, but the discussion and planning could be done by email. It was felt important that the revision should be started immediately. TD suggested that the Division VIII Advisory Subcommittee should be activated for commenting or assisting with the task.

> ***Action:** RSL will prepare a first draft of the contents and distribute it to the whole Division. ATH to ask for interest for participating in a subcommittee, which would form a Task Group and Editorial Board.

11.3. UVCB nomenclature for industrial chemicals and the impact of ECHA on nomenclature for the registration of substances that are intentionally produced as complex mixtures of chemicals

MMR described the need for having proper nomenclature for industrial chemicals (see also Item 9 in the current minutes and Item 12.4 of the 2018 Basel minutes). If ECHA were interested, there was the possibility to establish a project.

***Action:** MMR will contact ECHA to establish if there was any interest.

11.4. Proliferation of IUPAC terminology to denote that names are (maybe) acceptable (recommended, retained, preferred, alternatively used, sometimes used, widely used, etc.) or not acceptable (not recommended, (strongly) discouraged, not included in these recommendations, deprecated, etc.) or to characterise them otherwise (common, traditional, trivial, etc.)

The problem of having too many different categories of names ('approved', 'systematic', 'provisional', *etc*.) was described in Item 12.5 of the 2018 Basel minutes. Since this is a question of terminology, TD had sent a document to ICTNS highlighting the problem. *PAC* used defined terminology and we might be constrained by this. Therefore, there should be no action for now. It was noted that in any case, this was not a project but rather an activity.

11.5. Revision of Principles of Chemical Nomenclature

GJL reported that the second edition of *Principles* was published in 2011, edited by GJL but with individual chapters written by ten individuals. Since then there had been developments in a range of areas such as PINs and InChIs. A new *Blue Book* had been published with corrections and revisions about to appear. The latest *Red Book* was published in 2005 with its revision underway. Consequently, there have been new recommendations that were not considered in the *Principles* of 2011. Other recommendations, such as the proposal for modification of end-of-line hyphenation and also the uses of kappa in both organic and inorganic names, needed to be presented to the world in easily assimilable terms.

A possibility might be to formulate this as an IUPAC project, in order to fund at least one meeting for all the contributors. GJL said he believed that as nomenclature became broader and more complex, the popular expositions of IUPAC recommendations, such as *Principles* and the *Brief Guides* should become a regular aspect of IUPAC activities.

In the ensuing discussion, it was agreed that the revision of *Principles* should run concurrently together with the *Red Book*, kappa and Alignment projects, but it should still be a separate project. The outstanding nomenclature issues should be clear before a new *Principles* was published (resolution of concepts such as kappa, Alignment project outcomes, metallacycles, *etc.*). There was also discussion about the possible need for a book such as *Fundamentals of Chemical Nomenclature*, which would be less comprehensive than *Principle*s, but more detailed than the *Brief Guides*. The benefits of having a PDF version and a mobile application over the printed book was also discussed.

***Action:** GJL will approach the RSC to obtain a copy of the final electronic document for easy modification. A Task Group will be formed.

11.6. Other projects

11.6.1. Constitutional dynamic polymers (dynamers)

JV mentioned that Division IV had been considering in Paris to submit a project proposal on dynamers. Supramolecular phases fall under this theme. Nomenclature recommendations for supramolecular species (hydrogen bonding, pi-stacking, secondary bonding interactions) were much

needed. One possibility would be to apply source-based nomenclature. Since there was no change in the name of the unit when only supramolecular species were formed, it was not clear how these kinds of situations should be handled in chemical nomenclature. ATH noted that the polymer people were the experts and would be best placed to judge the need for such nomenclature. He also remarked that a project should not be started just for the sake of starting a project.

11.6.2. Brief guide on biochemical nomenclature

TD had suggested a project on *Essentials of Biochemical Nomenclature* in the meeting of JCBN. It might be worthwhile to have a four-page brochure as a companion to the other *Brief Guides*. There was no need for any action now by the Division Committee, other than that given below.

> ***Action:** TD will compile a list of possible topics for inclusion in a *Brief Guide* concerned with biochemical nomenclature.

11.6.3. Enhanced recognition and encoding of stereoconfiguration by InChI tools

AY proposed a project for the enhanced recognition and encoding of stereoconfiguration by InChI tools. InChI and InChIKey were already very useful for identification and searching of substances in various sources of chemical information. Some types of stereoisomerism and representations of stereoconfiguration were not recognized by the InChI system. Unsupported stereoisomerism types resulted in the inability to distinguish specific isomers, and the incorrect treatment of some representations resulted in incomplete or even wrong InChI identifiers.

The project also intended to address non-tetrahedral stereoconfigurations, which were often encountered not only in coordination compounds but also in organic compounds, as well as unrecognized configurations for several specific cases including pyramidal arrangements and cumulenes with more than three cumulated bonds.

> ***Action:** AY will propose and formulate the nomenclature parts of this project.

12. IUPAC nomenclature consultancy/naming service/contact addresses for users, *etc.*

The contact form on the IUPAC webpage offered the possibility to enquire about nomenclature problems, but it was not clear how such requests should be handled. Currently, the enquiries were addressed by the Secretariat to the President of Division VIII. If ATH cannot supply suitable answers, he will pass the enquiry to other members of the Division Committee, who in his judgment might be able to provide help.

13. Membership matters

MMR informed the meeting that because of the advent of GDPR in Europe, all email addresses on the IUPAC website were private unless specifically agreed by the individuals that they could be made public.

> ***Action:** All members of Division VIII need to go to the IUPAC Division VIII webpage and make their email addresses public.

It was also decided that the representatives of CAS and CCDC should be permanent *ex officio* members on the Division VIII committee.

13.1. Status of Division VIII Committee membership 2020–2021

The Division VIII roster for the biennium 2020–2021 is shown in Appendix 5. ATH informed the Division Committee members that Leah McEwen (LME) had suggested that InChI Subcommittee officers should be made *ex officio* members of Division VIII. The proposal to include Subcommittee Chairs on the Division roster was discussed and approved (see also Item 7).

> ****Action:*** Subcommittee Chairs will be included on the Division VIII roster as *ex officio* Committee Members. ATH will contact LME.

13.2. Division VIII representatives in other IUPAC bodies

Division VIII has representation on (or members of the Division Committee are members of) the following bodies:

CCE:	RM is the representative from Division VIII
PAC Editorial Advisory Board:	KHH is the representative from Division VIII (ATH in his absence)
ICTNS:	TD is the representative from Division VIII
COCI:	MMR is a Member of COCI and thus also the contact person for Division VIII
JCBN:	GPM is the Chair, APR and TD are Associate Members, and ATH is *ex officio* a Member. Gareth Owen is a new IUPAC-funded Titular Member of JCBN as a replacement for Marcus Ennis, who resigned early in 2018.
CPCDS:	KTT and AY are members of the Subcommittee on Cheminformatics Data Standards (SCDS); Leah McEwen (LME) is the Chair of this subcommittee.

13.3. Division VIII Advisory Subcommittee

The list needs to be updated. After some discussion of the dormant nature of the Division Advisory Subcommittee a decision was made to involve the subcommittee more actively in the affairs of the Division.

> ****Action:*** RSL will write to the subcommittee members, send them the approved minutes of the 2018 Basel Division Committee meeting, and enquire how they would like to serve (whether to receive draft documents, participate in developing nomenclature, or in some other way). In addition, the membership of this subcommittee needs to be updated and reviewed.

14. Publicity

14.1. Division VIII (and related) publications since the 2018 Division Committee meeting

See list of publications in Appendix 6.

14.2. IUPAC-IUBMB nomenclature website

GPM no longer has access to the usage information or statistics on this website. Otherwise, this website is very useful and apparently well-used (https://www.qmul.ac.uk/sbcs/iupac/).

14.3. IUPAC website

It was felt that the IUPAC website had improved, but the search function was still difficult. Proper links to projects are still missing.

15. Any other business

15.1. Visit by President, Vice-President and Secretary-General of IUPAC

The IUPAC Officers Qi-Feng Zhou (President), Christopher M.A. Brett (Vice-President) and Richard M. Hartshorn (Secretary-General) visited the Division Committee meeting. The main discussion was centered on the curtailment of the 'off-year' Division meetings. While the financial problems of IUPAC were clearly understood, it was generally felt that nomenclature, in particular, needed annual face-to-face meetings. If there were such meetings only during General Assemblies, when there were also conflicts with the meetings of other IUPAC committees, the nomenclature work would be much slower in producing any outcomes. TD noted that if the objective was to save money, it did not make sense for the whole Division Committee to travel to distant locations, where GAs were often held. He proposed that the Division Committee should meet at locations which minimized expenses, and then only the Division President would go to the GA to report on the work of the Division. RMH noted, however, that there was merit in having different Divisions meeting together during the GA.

> ***Action:** RMH invited Division VIII to produce a paper highlighting their views. ATH agreed to provide a paper outlining the Division's opinion.

15.2. Reports from cross-over meetings

15.2.1. Divisions II & VIII

Division VIII members: MAB, NB, ATH, RSL, GJL, RM, EM, LM, EN, MAP, MMR, MAS, ES, CT, AY

Several topics were briefly discussed and liaisons were decided:

- Neil Burford will be the liaison for the Division II project *'Terminology guidelines and database issues for topology representations in coordination networks, metal-organic frameworks and other crystalline materials'* (2014-001-2-200, Chair: Lars Öhrström; see Item 10.8).
- A new collaborative project (between IUPAC and I) concerning inorganic nanoscale particles was being initiated. The Division VIII members of the Task Group were ECC, RMH, AY, and MAB. The current ISO member was Scott Brown, but this will be complemented later with additional ISO personnel. This collaboration will, in fact, consist of two discrete projects: carbon nanotubes, which was already underway, and inorganic clusters, for which the Task

Group was currently being assembled. There was a need for Division II representation and Önder Metin was appointed in this Task Group.

- The revision of *Red Book 2005* was about to begin. The Task Group was yet to be formed in Division VIII, but the Division II representatives would be Robin Macaluso and Jan Reedijk.
- The complete revision of the *Gold Book* was discussed. Both Divisions had been informed that the planned schedule for the revision was two years. Since this involved complete revision of both the database and the content, which comprised both recommendations and definitions of terms, this schedule was not considered realistic. It was thought that possibly the Young Observers of IUPAC could be involved in this work (see Item 15.3).
- The collaborative project '*Terminology and nomenclature of inorganic and coordination polymers'* ('TINCOPS', 2011-035-1-800, acting Chair: Lars Öhrström; see Item 10.13) was progressing. While TD was already a Task Group Member, Clare Tovee will join the project as further liaison between the Divisions.

15.2.2. Divisions IV & VIII

Division VIII members: MAB, ATH, RSL, GJL, EN, MMR, CT, JV, AY

- ATH informed the meeting about the situation concerning KHH.
- The outstanding collaborative projects (see Items 10.19.1 – 10.19.8) were reviewed and it was concluded that there were no major problems. The projects listed as Items 10.19.6 – 10.19.8 were already published, and the other projects were near to completion.
- The 'Agrico' project was currently going through the proposal approval process. JV was the Division VIII representative on SPT responsible for nomenclature.
- There was a need to increase the precision of indicating the repeating units. This would be a mixed project involving both terminology and nomenclature. JV was the Division VIII representative.
- AY reported that there was a need for electronic representation of polymeric structures. The graphical representation would be the critical part of this approach. This project will be discussed in SPT and decisions will be made at a later date – a proposal will be submitted next year.
- A follow-up to the 'STAR' project was being planned. JV and possibly GPM would stand in for KHH while he was indisposed.
- The project 'Nanonano' will be about lithography and polymers. It will have connections with the Division VIII projects on carbon nanotubes and inorganic nanoparticles and AY and JV will represent Division VIII.
- The revision of the *Polymer Brief Guide* was discussed. The need was to include basic terms. The manuscript (a two-page document) had been written and could be submitted in 2020.
- ATH described the upcoming revision of the *Red Book*. It will also contain a section on coordination polymers. He also mentioned the possibility of a future revision of the book *Principles of Chemical Nomenclature*.

15.3. Report on the ICTNS meeting at the GA in Paris

TD reported on the discussion of items from the ICTNS meeting that had taken place the previous day. There had been a detailed discussion about the procedures of ICTNS in order to solve problems with the documents. It had been concluded that some problems were not in the hands of ICTNS, since

the articles were handled by the publisher. Divisions had to be careful to submit only finalized manuscripts, which also took care of accepted language and punctuations. ICTNS had also emphasized that Divisional review was a serious matter. It was assumed that the Divisional representative on ICTNS looked at all documents submitted by the Division.

There had also been discussion about the revision of the *Gold Book: Glossary of Chemical Terminology*. Each Division would be responsible for their own entries. Division VIII was responsible for *ca.* 280 entries. These are terms in our Recommendations that need to be defined. The checking necessitates going back to the original Recommendations to see that they are correct and up-to-date. The International Younger Chemists Network (IYCN) might be asked to contribute to this task under the mentorship of a Division member. See project details under Item 10.22.

15.4. Speed networking

There would be a 'speed networking' event in the evening of Tuesday 9 July bringing together the Divisions and Young Observers. After this, there would be a poster presentation. Division VIII had two posters to present: the *Inorganic* and *Organic Brief Guides*. It was decided that AY would present the former and MMR the latter. It would be the first public exposure for the yet-to-be-published *Organic Brief Guide*.

16. Dates and venue for next meeting

As a result of financial constraints, IUPAC now expected 'off-year' meetings to be carried out online. If Task Group Chairs wrote reports on their projects before the Division Committee meeting, these could be circulated, thus shortening the time needed for the meetings. Task Groups that had funds available for a physical meeting could meet at around the same time and participate in the Division Committee meeting online. No decisions could be made at this time, but Copenhagen was proposed as a tentative venue for the meeting, which could possibly be held at the end of August.

17. Adjournment

ATH thanked the participants for their attendance and contributions, and a group photograph was taken (see Appendix 1). The meeting was adjourned at 12h30 on 7 July.

Appendix 1

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Membership - Division (VIII)

Chemical Nomenclature and Structure Representation

2018 - 2019

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

11 October 2017

Attendees at Division Committee Meeting, Paris, France, 6 – 7 July 2019

From left to right: Mike Beckett, Ture Damhus, Risto Laitinen (Secretary), Andrey Yerin, Alan T. Hutton (President), Clare Tovee, Jeffery Leigh, Maria Petrova, Michelle Rodgers, Molly Strausbaugh, Ebbe Nordlander, Elisabeth Mansfield, Jiří Vohlídal, Erik Szabo

Not in photo: Neil Burford, Richard Hartshorn, Steve Heller, Robin Macaluso, Ladda Meesuk, Gerry Moss, Amelia Rauter, Young Observers, IUPAC Officers

Appendix 2.

International Union of Pure and Applied Chemistry
Division VIII
Chemical Nomenclature and Structure Representation

Draft agenda for Division Committee Meeting
Paris, France, 6–7 August, 2019
Venue: **Palais des Congrès, Room 326/7M**

Schedule

Saturday, July 6		***Sunday, July 7***	
09.00 am - 10.15 am	DC meeting	 08.00 am - 09.00 am 09.15 am - 10.15 am	Cross-over meetings: Divs. VIII - II (Room 326/7M) Divs. VIII - IV (Room 351)
10.15 am - 10.35 am	Coffee break	10.15 am - 10.35 am	Coffee break
10.35 am - 11.30 am 11.30 am - 12.30 pm	DC meeting Joint meeting with InChI Subcommittee	10.35 am - 12.30 pm	DC meeting
12.30 pm - 01.30 pm	Lunch	12.30 pm - 01.30 pm	Lunch
01.30 pm - 03.00 pm	DC meeting	01.30 pm - 03.00 pm	DC meeting
03.00 pm - 03.20 pm	Coffee break	03.00 pm - 03.20 pm	Coffee break
03.20 pm - 05.30 pm	DC meeting	03.20 pm - 04.30 pm	DC meeting

Agenda

1. Welcome, introductory remarks and housekeeping announcements

2. Attendance and apologies

3. Introduction of attendees

4. Approval of agenda

5. Approval of minutes of meeting in Basel, 13–14 August 2018

6. Matters arising

7. Division Rules

8. Division VIII Emeritus Fellows Program

9. Interactions between Division VIII and other (IUPAC) bodies in relation to documents and projects involving chemical nomenclature.

10. Reports of Division VIII projects

10.1. Building Broader and Deeper Links Between OPCW and IUPAC (proposal 2018-022-2, Richard Hartshorn)

10.2. Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature (2017-033-1-800, Karl-Heinz Hellwich)

10.3. Graphical representation standards for chemical reaction diagrams (2003-045-3-800/2012-033-1-800/2017-036-2-800, Keith T. Taylor)

10.4. IUPAC International Chemical Identifier (InChI) projects

- *10.4.1. InChI extension for mixture composition (2015-025-4-800, Leah McEwen)*
- *10.4.2. Identifying International Chemical Identifier (InChI) Enhancements – QR codes and Industry Application (2015-019-2-800, Richard Hartshorn)*
- *10.4.3. Implementation of InChI for chemically modified large biomolecules (2013-010-1-800, Keith Taylor)*
- *10.4.4. Handling of Inorganic Compounds for InChI V2 (2012-046-2-800, Richard Hartshorn and Hinnerk Rey)*
- *10.4.5. Redesign of Handling of Tautomerism for InChI V2 (2012-023-2-800, Marc Nicklaus)*
- *10.4.6. InChI requirements for Representation of Organometallic and Coordination Compound Structures (2009-040-2-800)*
- *10.4.7. InChI Open Education Resource (OER) (proposal 2018-012-2, Robert Belford)*

10.5. Corrections, Revisions and Extension for the Nomenclature of Organic Chemistry - IUPAC Recommendations and Preferred Names 2013 (the IUPAC Blue Book) (2015-052-1-800, Karl-Heinz Hellwich)

10.6. Nomenclature of carbon nanotubes and related substances (2013-056-1-800, Elisabeth Mansfield)

10.7. End-of-line hyphenation of systematic chemical names (2014-003-2-800, Albert Dijkstra)

10.8. Terminology guidelines and database issues for topology representations in coordination networks, metal-organic frameworks and other crystalline materials (2014-001-2-200, Lars Öhrström)

10.9. Nomenclature for metallacycles containing transition metals (2013-030-1-800, Alan Hutton)

10.10. Nomenclature for polyhedral boranes and related compounds (2012-045-1-800, Michael Beckett)

10.11. Revision and extension of IUPAC recommendations on carbohydrate nomenclature (2012-039-2-800, 2015-035-2-800, 2017-026-1-800 Johannes Vliegenhart)

10.12. A comparison of assignment of hydro prefixes, added and indicated hydrogens in IUPAC, CAS and Beilstein nomenclature systems (2012-037-1-800, Andrey Yerin)

10.13. Terminology and nomenclature of inorganic and coordination polymers (2011-035-1-800, Richard Jones); for short TINCOPS

10.14. Brief guides to the nomenclature of organic and inorganic chemistry ('Essentials' of organic and inorganic nomenclature) (2010-055-1-800, Richard Hartshorn and Karl-Heinz Hellwich)

10.15. Glossary of small molecules of biological interest (2009-022-2-800, Marcus Ennis)

10.16. Nomenclature of flavonoids (2009-018-2-800, Amelia Rauter)

10.17. Preferred names for inorganic compounds (2006-038-1-800, Ture Damhus)

10.18. Nomenclature of phosphorus-containing compounds of biochemical importance (2006-019-1-800, Gerard Moss)

10.19. Polymer projects (with Division IV)

- *10.19.1. Graphical Representation of Polymer Structures (2017-039-2-800, Karl-Heinz Hellwich)*
- *10.19.2. Nomenclature for polymeric carriers bearing chemical entities with specific activities and names (2014-034-2-400, Michel Vert)*
- *10.19.3. Strucure-based Nomenclature for Regular Linear, Star, Comb and Brush Polymers (2013-031-3-800, Jiazhong Chen)*
- *10.19.4. Definitions and notations relating to stereochemical aspects in polymer science (2009-047-1-400, Karl-Heinz Hellwich and Graeme Moad)*
- *10.19.5. Revision of IUPAC Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology (2008-020-1-400, Philip Hodge) (Web-based IUPAC recommendations on polymer nomenclature)*
- *10.19.6. Preferred names for polymers – a list of preferred, acceptable (other IUPAC-approved) and not acceptable (ambiguous, wrong or outdated) names for polymers (2008-015-1-400)*
- *10.19.7. Guidelines for abbreviating polymer names (2006-004-1-400)*
- *10.19.8. Terminology and structure-based nomenclature of dendritic and hyperbranched polymers (2001-081-1-800, Alain Fradet and Jaroslav Kahovec)*

10.20. Survey of Definitions and Use of Common Solid-State Chemistry terminology (2015-053-1-200, Robin Macaluso)

10.21. Nomenclature of Homodetic Cyclic Peptides Produced from Ribosomal Precursors (2015-003-2-300, Martin Reaney)

10.22. IUPAC Color Book Data Management (proposal 2013-052-1, Kinnan)

10.23. Rules for Abbreviating Protecting Group (2011-044-1-300, Margaret Brimble)

11. Future projects/activities

11.1. International Standards Organization (ISO) liaison. Nanoparticles projects (c.f. item 10.6).

11.2. New edition of Nomenclature of Inorganic Chemistry, the 'Red Book'.

11.3. UVCB nomenclature for industrial chemicals and the impact of ECHA on nomenclature for the registration of substances that are intentionally produced as complex mixtures of chemicals.

11.4. Proliferating IUPAC terminology to denote that names are (maybe) acceptable (recommended, retained, preferred, alternatively used, sometimes used, widely used, etc.) or not acceptable (not recommended, (strongly) discouraged, not included in these recommendations, deprecated, etc.) or to characterise them otherwise (common, traditional, trivial, etc.).

11.5. Other projects.

12. IUPAC nomenclature consultancy/naming service/contact addresses for users *etc.*

13. Membership matters

13.1. Status of Division VIII Committee membership (see current and 2020-2021 membership rosters in Appendix)

13.2. Division VIII representatives in other IUPAC bodies CCE, PAC Board, ICTNS, COCI, JCBN

13.3. Division VIII Advisory Subcommittee

14. Publicity

14.1. Division VIII (and related) publications since the 2018 Division Committee meeting

14.2. IUPAC-IUBMB nomenclature website

14.3. IUPAC website

15. Any other business

16. Dates and venue for next meeting

17. Adjournment

Appendix 3

Division VIII
Chemical Nomenclature and Structure Representation

DIVISION RULES
(Draft, March 2019)

Preamble

The following document is a considerably revised and expanded version of the 2005 archive material. It should serve to provide some orientation for new members of the Division, and will support Division Officers in the discharge their responsibilities. The document has three sections: the first, *General Division Rules,* is based largely on the relevant IUPAC Statutes and Bylaws, with particular modifications reflecting current practice in the running of Division VIII. The second section is a collection of *Terms of References* that are specific for Division VIII and includes material relevant to InChI and JCBN. Finally, there is a *List of Abbreviations* to help the novice interpret the enigma of IUPAC code. This Division Rules document is a living text which is expected to evolve and to be refined through discussion at future Division meetings.

TABLE OF CONTENTS

A. General Division Rules

1. Mission

The mission of the Chemical Nomenclature and Structure Representation Division is to maintain and develop standard systems for designating chemical structures, including both conventional nomenclature and computer-based systems.

This mission is accomplished by the following **strategy**:

(a) Identify the needs of the user community.
(b) Generate projects arising from those needs.
(c) Identify project leaders and Task Groups to carry out the work.
(d) Administer approved projects financially, monitor their progress, and approve resulting recommendations for review by established IUPAC procedures.
(e) Identify new sources of expertise and enable their involvement in projects.
(f) As far as possible, ensure that nomenclature systems, projects and the resulting recommendations are compatible with each other, with established IUPAC recommendations, and with computer-based systems for manipulating chemical names and structures.

2. Division Committee

Under the Statutes, Bylaws, and Policies of the Union (see https://iupac.org/wp-content/uploads/2018/08/Statutes-and-ByLaws-2017.pdf), the Division is managed by its Division Committee. Statute S10 (Divisions and Commissions) and Bylaw B3.1 (Division Committees) and their subsections are particularly relevant.

(a) Tasks

The Division Committee is responsible for initiating and managing scientific projects, symposia and other activities within its area of responsibility, and for cooperating with other Divisions and Standing Committees (especially ICTNS) in initiating and managing interdisciplinary projects, symposia and other activities.

The Division Committee appoints two of its members to act in the portfolios of Project Manager and Web Manager, to coordinate and monitor activities in these areas.

The Division Committee approves the Recommendations and Technical Reports that are submitted to ICTNS for publication in *Pure & Applied Chemistry*; it is the responsibility of the Division President to ensure that this happens.

It is the responsibility of the Division Committee to disburse the biennial funding allocated by IUPAC for support of Division-associated Projects and operating expenses. Toward this end, the DC facilitates the initiation of new Projects, monitors the management of ongoing Projects, and participates in processing Project outcomes.

In addition to its Project-related activities, the DC makes recommendations to the IUPAC Bureau with regard to IUPAC endorsement of scientific meetings.

The DC may award 'IUPAC Division VIII Emeritus Fellow' status to selected individuals. Terms of reference for the 'Division VIII Emeritus Fellows' programme are specified below in Section B1.

(b) Composition

The Division Committee comprises members with appropriate expertise as follows (Bylaw B3.1.4):

- No more than ten Titular Members (including all Officers as defined below)
- No more than six Associate Members
- No more than ten National Representatives

(c) Membership and appointments

Titular Members (TMs) of the Division Committee are chosen by an electorate comprising the current Division Committee, Task Group Chairs of active projects and members of the current and previous Nominating Committee, from a ballot put together by the Nominating Committee (see below). When elected, they serve for a term of two years, and may be re-elected for a further two years, but the term of service shall be not be more than four consecutive years, and shall cease on election as an Officer.

Associate Members (AMs) are selected by the Division Executive Committee for a term of two years, with the possibility of re-appointment consecutively for two more years only.

National Representatives (NRs) are selected by the Division Executive Committee on nomination by the National Adhering Organizations for a term of two years, with the possibility of re-nomination and re-appointment consecutively for two more years only.

Interim appointments to fill vacancies on the Division Committee occurring between meetings may be made by the Division President, after consultation with the other Division Officers, for a term ending at the end of the year in which the next General Assembly is held. Interim appointments are subject to approval by the IUPAC Bureau or IUPAC Executive Committee.

Provision is made for removal of Division Committee members who are unable to perform the expected duties and/or who do not participate at the levels expected for their particular type of membership. Further details are given in Section B2 below.

3. Officers and Executive Committee

The Officers of the Division are elected from existing or new TMs by the Division Committee, subject to final approval by the Council, and comprise the Division President, the Division Vice-President or Division Past-President, and the Division Secretary.

(a) The Division President is the administrative head of the Division, takes care of the biennial Division budget, presides at meetings of the Division Committee, and is an *ex officio* member of all bodies of the Division. The President serves as a member of the IUPAC Bureau and is the principal representative of the Division within and outside the Union.

(b) The Division Vice-President or Past-President acts for the President in his or her absence and assists the President as requested. The Vice-President or Past-President shall assume the office of Division President in the event of the President being unable to perform the functions of that office, without prejudice to the forthcoming period of office as President, subject to the terms of Bylaw B3.1.4.
(c) The Division Secretary assists the Division President in carrying out the business of the Division and maintains the records of the Division.
(d) The Officers together form a Division Executive Committee to act for the Division Committee between meetings.
(e) The **terms of office** of the Officers of the Division are, subject to the limitations in Bylaw B3.1.4, as follows:

The Vice-President is President-Elect and serves a term of two years, then assuming the office of President for a maximum term of four years. At the end of the President's term he or she becomes the Past-President for a term of two years. Thus, for the first two years the President is assisted by the Past-President and for the last two years the President is assisted by the Vice-President. The Division therefore has either a Vice-President or a Past-President, and not both at the same time.

The Secretary serves a term of four years and is eligible for re-election to a second term of four years.

4. Nominating Committee

Candidates for election to Titular Membership of the Division are selected (based on a submitted CV) by the Nominating Committee from nominations that have been received by the Secretariat, as prescribed by IUPAC policy and procedures defined by the Bureau:

(a) The Nominating Committee consists of five members including the chair (subject to an exception by the Bureau), with no more than two members from the existing Division Committee and the other three chosen based on the breadth of their expertise. The Division President will not be a member of the Nominating Committee.

(b) The Nominating Committee and its chair are appointed by the Division President with the approval of the Secretary General.

(c) Categories of vacancies may be established by the Division Committee, in order to ensure diversity in subject matter, geographic and gender distribution, or other characteristics. More than one nominee for each vacancy is highly desirable but not mandatory. If there is only a single candidate for a vacancy, the Nominating Committee must submit a justification to the Secretary General. Candidates need to agree to be nominated and must have submitted a CV to the IUPAC Secretariat.

5. Elections

Elections of TMs shall be conducted by the members of the Division Committee by e-mail under procedures defined by the IUPAC Secretariat.

TMs shall be chosen by an electorate comprising the TMs, AMs and NRs on the Division Committee, together with the members or officers of such other bodies within the Division that

the Bureau may specify IUPAC (Bylaw B3.1.4). TM candidates are nominated by the Nominating Committee.

AM candidates are nominated by the Division Committee and selected by the Division Executive Committee.

NR candidates are nominated by the National Adhering Organizations. The list of nominees is sent via the IUPAC Secretariat to the Division Nominating Committee. Each Adhering Organization may have no more than one NR in the Division Committee.

Division Officers will generally be selected at a Division meeting or by e-mail, with TMs, AMs, and NRs eligible to participate. If there is no clear consensus, a vote should be taken among the TMs, AMs, and NRs. The candidates for Vice-President (President-Elect) and Division Secretary would recuse themselves from this process.

Subcommittee Chairs (SCCs) are selected by their respective constituencies. A SCC should be a TM where possible. While not mandated, it is recommended that these posts are reviewed by the SC at least every four years, and that SCCs do not serve for consecutive terms longer than four years. Recommendations for these posts are forwarded to the DC for final approval whenever such selections are undertaken.

6. Division Budget

The Division receives a biennial budget from IUPAC. The budget is administered by the Division President. About 70% of the budget should be used for projects, and about 30% can be used for administrative matters, primarily to cover travel expenses in connection with Division Meetings. Uncommitted budget goes back to IUPAC at the end of a biennium.

7. Projects

In accordance with the IUPAC Project Guidelines, project applications can be made by chemists around the world, but in most cases projects are initiated by members of the Division. Projects should be related to the needs of the global scientific community and usually result in Recommendations or Technical Reports. Original research is not supported. Project applications go through internal and external review processes conducted by the IUPAC Secretariat. The Division Committee appoints one of its members as Project Manager to coordinate and monitor the submission, progress and outputs of the Division's Projects.

8. Meetings and Communication

There is one Division Committee (DC) meeting per year. In years of the IUPAC General Assembly (GA), these meetings take place during the GA. The meetings of the GA are confirmed by the IUPAC Council with regard to venue and date two years in advance, during the preceding meeting of the GA. In other years, meetings are denoted as 'off-year' meetings. When selecting the venue for the off-year meeting of the DC, overall travel costs must be taken into account. Both GA and off-year DC meetings will usually be preceded by several days of Task Group meetings for the various Division projects.

Barring unavoidable circumstances or critical scheduling conflicts, TMs are expected to attend all DC meetings and to participate fully in DC activities as appropriate, including reviewing of IUPAC Project applications and applications for IUPAC endorsement of conferences. TMs will

receive reimbursement of their travel expenses to the annual meetings either from the IUPAC Secretariat (GA meetings) or from Division VIII funds (off-year meetings). Pending the availability of Division or Project funding to assist with travel expenses, and barring unavoidable circumstances or critical scheduling conflicts, AMs and SCCs are likewise expected to participate fully in DC activities as appropriate. While it is hoped that NRs will also be able to attend the DC meetings and to engage actively in various DC activities, it is appreciated that such participation may be difficult without a funding line available to assist in covering the associated expenses. However, NRs are expected to be conversant on all DC topics and to offer input as appropriate by e-mail correspondence. It is current Division VIII policy to fund attendance of SCCs at official DC meetings.

In addition to the TMs, AMs, NRs, and SCCs, the DC may invite *ad hoc* participation of selected individuals who are not DC members for expert input during its deliberations and to contribute to discussion of its decision-making responsibilities, but these non-DC members will not be eligible to vote on any Division issues.

Between meetings, communication within the Division Committee proceeds as needed by e-mail and by internet-based conferences.

9. Subsidiary Bodies

(a) The Division Committee may establish and the Division President may appoint subsidiary bodies, such as subcommittees, working parties and advisory groups, which will all have the status of Division subcommittees, as described in Statute S10.6. The terms of reference or charge to each group, as well as its lifetime, shall be established by the Division Committee, and this information must be submitted to the Secretariat.

Current Subcommittee of Division VIII is (year 2019):
InChI Subcommittee

(b) The Division Committee may propose to the Bureau the establishment of Commissions, with terms of reference and lifetimes, under the provisions of Bylaws B3.1.7.5 and B3.3.

Current Commission of Division VIII is (year 2019):
IUBMB-IUPAC Joint Commission on Biochemical Nomenclature (JCBN)

(c) Task Groups may be formed to carry out specific Projects (see Section 7 above) under general IUPAC policies for the conduct of Projects.

(d) The Division Executive Committee will exercise responsibility and oversight over all bodies created under parts (a), (b) and (c).

(e) Terms of reference for the above Subcommittee and Commission may be found below in Sections B3 and B4.

10. Amendments

These Rules may be amended by the Division Committee, subject to approval by the Council.

B. Terms of Reference for Division-Specific Activities

1. Terms of Reference for the *'Division VIII Emeritus Fellows Programme'*

This category of membership will be bestowed upon meritorious individuals who have *earned by service* a special recognition *upon their retirement* (departure) from one or more Division VIII administrative posts or from a multiple of key Division VIII Project roles. While Division VIII Emeritus Fellow (EF) membership will typically be granted to individuals who have reached a point in their careers where they are beginning to diminish their involvement in professional activities, this is not a requirement of the award. Thus, EFs can still hold future IUPAC posts and can participate in future IUPAC Projects.

Privileges

1. A standing invitation to attend Division and Subcommittee Meetings appropriate to the EF's technical background.
2. The possibility to receive a reimbursement for a portion of travel costs incurred while attending a Division Meeting, particularly when the meeting is associated with an IUPAC General Assembly and World Chemistry Congress. This possibility and the level of actual reimbursement will be determined by the Division Committee (DC) prior to such meetings, taking into account the status of the budget of the Division at that point in time, the anticipated overall costs for the meeting, and the number of EFs who have expressed a desire to attend.

Obligations

1. Regular (biennial) renewal of membership; immediate update of contact information upon any change.
2. Willingness to serve as an advisor, referee or consultant, according to the EF's own schedule, if called upon by the Division or by any other IUPAC body.

Selection and Appointment

1. Recommendation of individuals for EF membership can be put forward by any DC member (TM, AM, NR) or SCC after using whatever mechanisms they choose to identify candidates within their own ranks. However, candidates must be made aware of their selection for such and, in turn, agree to the aforementioned obligations should they be appointed.
2. Recommendation packets will be forwarded via e-mail attachment to the Division President and Secretary. Packets will include (a) a one-page summary of why the candidate is meritorious and deserving of EF status, and (b) the curriculum vitae of the candidate.
3. Nomination packets will then be forwarded to the entire DC by the Division President and Secretary.
4. Consideration of nominees and appointments will be undertaken annually during a DC meeting.
5. Notification of the outcome will be provided to each candidate by the Division President. Only the list of appointed EFs will appear in the public record.

Numbers of Emeritus Fellows
The total number of EFs will not be capped. However, in order to preserve the meritorious nature intended for this prestigious category of IUPAC Div VIII membership, no more than three such awards will be bestowed in each Biennium, and not more than one from each Subcommittee or Commission.

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2. Procedures for removal of non-performing members
Division Committee members who are unable to perform the expected duties and/or who do not participate at the levels expected for their particular type of membership may be designated as *'non-performing members'*. The two most common examples of non-performance that have arisen are failure to respond to e-mail communications, and failure of TMs to attend scheduled meetings. Thus, these two areas, in particular, are further described below relative to prompting a need to remedy the situation at the DC level:

(1) Failure to respond to e-mails after three months, assuming that additional modes of contact (*e.g.*, telephone) have also been attempted subsequent to having e-mails sent twice (address verified to be correct by the Secretariat), and where these modes of communication were attempted over the course of at least one month; and
(2) Failure of TMs to attend two consecutive DC meetings without having a significant scheduling conflict, and likewise for AMs, NRs and SCCs when funding is being made available to assist them with their travel expenses.

Remediation
The President will provide a brief summary to the TMs and SCCs indicating why there is a need to place a particular individual into the category of a non-performing member. If there is a consensus among this group, then this same summary will be forwarded to the IUPAC Secretariat. If no objections are raised by the Secretariat, then a written letter from the Division VIII President will be sent to the individual indicating that his or her role on the DC is about to be terminated unless undue circumstances for their lack of performance can be cited in a reply letter that should be returned to the Division President within a one-month time period.

Unless such a reply letter is received, termination will occur automatically and the Division Executive Committee will undertake an interim appointment, or will become free to add a slot to its next membership ballot should an appropriate election time-point be drawing near.

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3. Terms of Reference for the *InChI Subcommittee*

Background
The IUPAC Division VIII InChI Subcommittee has the responsibility for continued authentication and development, in conjunction with the InChI Trust, of the IUPAC Chemical Identifier (InChI), the computer based chemical structure standard, and acts as the scientific advisory board to the InChI Trust. In turn, the InChI Trust develops and supports the non-proprietary InChI standard and promotes its uses to the scientific community.

Role of the InChI Subcommittee

- The IUPAC Division VIII InChI Subcommittee represents IUPAC's authority for recognition of the InChI standard.
- To act as a scientific advisory board for the InChI standard and to ensure the quality of the InChI standard and that it is aligned with community needs.
- To report back to the Committee on Publications and Cheminformatics Data Standards as well as Division VIII (https://www.inchi-trust.org/iupac/).
- To provide technical standard definitions and input to the InChI Trust, which develops and supports the non-proprietary InChI standard and promotes its uses to the scientific community. To consider and recommend modifications/extensions to the InChI standard.
- To review project proposals, any requests for change, define corresponding requirements and communicate these requirements to the InChI Trust with suggestions for prioritisation if necessary.
- To prepare recommendations, based on input from the working groups, IUPAC Project Groups and others for the future development of the InChI standard. To oversee the validation and periodic review of the code by ensuring appropriate procedures are in place to undertake timely validation/review events, receiving and considering outcomes, and monitoring the response to any recommendations from the working groups.
- To have oversight of, and report and make recommendations to the InChI Trust Board on the quality and applicability of the InChI standard. To report formally its proceedings, recommendations and matters of concern to the InChI Trust Board.
- To receive, consider and respond, as appropriate, to Minutes from the InChI Trust Board.

Make-up of the InChI Subcommittee

- To be decided by mutual agreement between the InChI Trust and IUPAC Div VIII.

Responsibilities of the InChI Subcommittee Chair and Secretary

- Sets the agenda for each meeting. (minimum frequency?)
- Ensures that agendas and supporting materials are delivered to members in advance of meetings.
- Makes the purpose of each meeting clear to members and explains the agenda at the beginning of each meeting.
- Encourages broad participation from members in discussion by calling on different people.
- Ends each meeting with a summary of decisions and assignments.
- Follows up with consistently absent members to determine if they wish to discontinue membership.
- Finds replacements for members who discontinue participation.

Responsibilities of the InChI Subcommittee Members

- Understand the goals, objectives and desired outcomes of the project.
- Understand and represent the interests of project stakeholders.
- Take a genuine interest in the project's outcomes and overall success.
- Act on opportunities to communicate positively about the project.
- Actively participate in meetings through attendance, discussion, and review of minutes, papers and other documents.
- Support open discussion and debate, and encourage fellow members to voice their insights.

4. Terms of Reference for the *IUBMB-IUPAC Joint Commission on Biochemical Nomenclature (JCBN)*

Composition and Terms of Office

1. The IUBMB-IUPAC Joint Commission on Biochemical Nomenclature is composed of four Titular Members, two appointed by IUPAC (including the Secretary) and two by IUBMB (including the Chairman), and up to eight Associate Members (appointed by JCBN itself).
2. The Chairman and the Secretary are each appointed for four years by the President of the appropriate Union, subject to whatever ratification is imposed by Union Statutes and Bylaws. JCBN may propose names of persons suitably qualified for appointment. The Chairman is *ex officio* a member of the IUPAC Division VIII Committee (Chemical Nomenclature and Structure Representation), with attendance at Division Committee meetings funded by IUBMB.
3. Candidates for Titular Membership may be proposed by the Commission. The Titular Members appointed by IUBMB shall also be Members of the Nomenclature Committee of IUBMB (NC-IUBMB).
4. The periods of service of the Titular Members and of the Associate Members are in accord with the Statutes and Bylaws of the appointing Union. The sum of the years of service as a Titular Member and as the Chairman or the Secretary must not exceed ten years.

Responsibilities

1. To maintain and develop naming systems for classes of natural product of interest to biochemists, especially steroids, amino acids and peptides, carbohydrates, lipids and nucleic acids.
2. To maintain and develop standards for symbolism to be used in databases for biopolymers.
3. To provide advice for biochemists on chemical names for compounds of biochemical importance.
4. To ensure that all recommendations are compatible with those issued by other nomenclature bodies of IUBMB and IUPAC.

Procedures

1. The Commission considers project proposals for work to be carried out under its own auspices, and forwards supported proposals to the IUPAC Secretariat and to the Chairman of IUBMB's Committee on Publications. Project review by IUPAC follows standard IUPAC procedures, involving assessment by external referees and by the appropriate Division Committee [normally the Division (VIII) of Chemical Nomenclature and Structure Representation]. Copies of all reviews obtained are sent to IUBMB, and agreement on approval and on level and distribution of funding is obtained by correspondence between IUBMB (via the Publications Committee Chairman) and the IUPAC Division VIII President. Approved projects are managed by the Commission.
2. Before recommending any resulting material for publication as an IUBMB-IUPAC document, the Commission should ensure that the fullest possible consultations have taken place and the widest possible consensus has been reached with the appropriate bodies of each Union: for IUPAC, the Division (VIII) of Chemical Nomenclature and Structure Representation and the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS); for IUBMB, the Nomenclature Committee (NC-IUBMB).

3. Approval to publish any material as an IUBMB-IUPAC document is to be obtained in the case of IUPAC from the IUPAC Division VIII Officers and ITCNS, and in the case of IUBMB from the Executive Committee of IUBMB.
4. The Commission normally holds an annual meeting concurrently with that of NC-IUBMB, and with the approval of the President of the IUPAC Division of Chemical Nomenclature and Structure Representation and the Executive Committee of IUBMB.
5. Associate Members will receive all documents of the Commission and their opinion will be sought by correspondence. An Associate Member may attend any meeting of the Commission, but his or her expenses will not be defrayed by the respective Executive Committee unless he or she has been invited as an observer under item 6.
6. The Commission is entitled to invite observers from similar bodies and experts in special fields to attend the meeting. The IUPAC Division President or the IUBMB Executive Committee should be asked in advance to defray any expenses that would arise from such an invitation.

C. Abbreviations

Relevant for Division VIII

AM	Associate Member (AM)
DC	Division Committee (DC)
DP	Division President (DP)
EF	Emeritus Fellow (EF)
NR	National Representative (NR)
PE	President-Elect (PE)
PP	Past-President (PP)
SC	Subcommittee (SC)
SCC	Subcommittee Chair (SCC)
TM	Titular Member (TM)
VP	Vice-President (VP)

Relevant for IUPAC (according to Bureau 2015)

BIPM	International Bureau of Weights and Measures
CCE	Committee on Chemistry Education
CCRF	Committee on Chemistry Research Funding
CHF	Chemical Heritage Foundation
CI	*Chemistry International*
COCI	Committee on Chemistry and Industry
CPCDS	Committee on Publications and Cheminformatics Data Standards
CPEP	Committee on Printed and Electronic Publications
CHEMRAWN	Chemical Research Applied for World Needs Committee
Div I	Physical and Biophysical Chemistry Division
Div II	Inorganic Chemistry Division

Div III	Organic and Biomolecular Chemistry Division
Div IV	Polymer Division
Div V	Analytical Chemistry Division
Div VI	Chemistry and the Environment Division
Div VII	Chemistry and Human Health Division
Div VIII	Chemical Nomenclature and Structure Representation Division
DP	Division President
EC	Executive Committee
EvC	Evaluation Committee
GA	General Assembly
IChO	International Chemistry Olympiad
ICSU	International Council for Science Unions
ICTNS	Interdivisional Committee on Terminology, Nomenclature and Symbols
IFCC	International Federation of Clinical Chemistry and Laboratory Medicine
IOCD	International Organization for Chemical Sciences in Development
IYC	International Year of Chemistry
MRC	Membership Relations Committee
NAO	National Adhering Organization
NC	Nomination Committee
NGO	Non-Governmental Organization
NICE	Network for Inter-Asian Chemistry Educators
OPCW	Organisation for the Prohibition of Chemical Weapons
PAC	*Pure and Applied Chemistry*
PC	Project Committee
SAICM	Strategic Approach to International Chemicals Management
STC	Standing Committee
STCC	Standing Committee Chair
TGC	Task Group Chair
TGM	Task Group Member
TM	Titular Member
VP	Vice President
WCLM	World Chemistry Leadership Meeting
YO	Young Observer

Appendix 4

InChI Trust Project Director's Report
January 2019

Summary:
In August 2018 Alan McNaught retired from the InChI project. Alan had been with the project from before it began when he and Ted Becker set up a meeting in Washington DC in 2000 to look into the matter of an IUPAC computer based chemical structure representation standard. Alan will be very solely missed for his dedication, competence, understanding of how IUPAC functions and to the creation and adoption of InChI.

Since the July 2018 report there continues to be good progress in many, but not all respects, with InChI and the InChI Trust. Specifically, three of the working groups have made considerable progress. The MInChI working group, led by Leah McEwan, has submitted the almost final specifications for programming the InChI algorithm for mixtures. In addition, the InChI OER (Open Education Resource) led by Bob Belford has started to make available a number of items for feedback and comment, including a draft of the taxonomy they plan to use. Lastly the newly formed isotopologues working group has made started to determine the needs and how to solve them for isotopes. Feedback to the initial version 1.00 of RInChI has been positive. Plans for what needs to go into version 2.0 have been started. More organizations, databases, and publications continue to use the InChI algorithm. Lastly, after a long period of no new Trust memberships, Google and OntoChem have joined the Trust for 2019.

Items covered in this report:
Membership/Support
InChI RFP/Contracts
InChI development and maintenance work
IUPAC InChI subcommittee and working groups
Meetings attended & Talks/ Posters given
Manuscripts
InChI Trust Web Site
InChI Usage
Technical Issues
Sustainability
Plans for 2019

Membership/Support:
There have been two new memberships since the last report – Google and Lutz Weber (OntoChem) have joined as Associate members starting in 2019. An initial interest and further email correspondence from the Chinese Chemical Society (CCS) will be part of the trip I will be taking to Beijing and Shanghai in May/June 2019.

As mentioned, numerous times in the past in most organizations, since InChI works and it is not high on their immediate priority lists, actual real progress is slow without a dedicated champion within an organization.
Elsevier and CAS have replaced their member representatives who will be attending the February 2019 Board meeting in Cambridge UK.
As of January 12, 2019
Existing Members and Associates: 17 (only 16 are listed on the web page)
Google & OntoChem will be added to the web site shortly to make the numbers 19 and 18 respectively
Supporters: 47

InChI RFP/Contracts

There have been no contract activities since the last report.

InChI Development & Maintenance Work

Igor Pletnev continues to do a superb and a very responsive job as the InChI programmer. With the release of version 1.05 there continues, as expected, to be useful feedback on minor issues and bugs as noted below. Gerd Blanke continues to do excellent work on the RInChI algorithm. An RFP for the MInChI programming is expected to be issued in early 2019. Bugs fixes and minor improvements to the algorithm will be released in version 1.051 in the spring of 2019.

Igor has reported that many people have been in contact with him regarding bugs, error, and issues with the algorithm. Without all this external help the algorithm would not be as good as it is.

Besides the inchi-discuss list, Igor had many valuable comments/issues, and advice reported in private correspondence by several experienced chemoinformaticians/developers which routinely use InChI, especially:
- Burt Leland (OpenEye)
- Dmitrii Tchekhovskoi (NIST)
- Daniel Lowe (NextMove)
- Karl Nedwed (BioRad)
- Gerd Blanke (StructurePendium)
- Andrei Yerin and Dmitry Redkin (ACD/Labs)
- Paul Thiessen and Evan Bolton (PubChem/NIH)

Also, there is a significant number of issues (and related fixes) Igor found in his own testing processes.
Some minor questions/reports also came from occasional InChI users, typically via Richard Kidd, and from other sources (like Google auto-fuzz).
In summary, we have many users and many people from all different areas of chemistry using and working to help improve the InChI algorithm.

IUPAC InChI subcommittee & working groups

InChI working Groups

As noted below, there are a good number of "working" groups which have been established over the past few years. I am beginning to believe the word "working" is not the correct word to use for a number of these activities. As we all know the effort that people have been putting in on these issues of extending the InChI algorithm are voluntary. They are not the person's day job for which they are paid. This leads to almost infinite differences in the progress being made (names omitted for obvious reasons). As a friend pointed out to me years ago, I feel like the caretaker at a cemetery. I have all these people below me, but no one listens to or obeys me. In some cases, people offered to help and discovered their task was not any easy one. In other cases, the leader of the group has not been a leader. In some cases, the "final" standard is still being debated year after year. As Confucius was believed to have said - "Better a diamond with a flaw than a pebble without". Put another way - perfection can paralyze. Or "Don't let the perfect be the enemy of the good." Remember what Dmitri did – essentially all by himself. He created the entire InChI algorithm! The "good" one is what Dmitrii did and it is this version of InChI that has and is being adopted and used at a furious pace. The bad news is that in doing "good" and not "perfect" there are things that need to be added and things that need to be improved. But please remember, if Dmitrii had to be perfect we would not be having this discussion. I implore those working groups which are close to being "perfect", stop, smell the roses, deliver version 1.0 (like we have done with InChI and RInChI, get feedback from the community and continue to improve. To quote Mao – This is the first step in a long march. Please, please take the first step.
We need to decide what to do with those enhancements that want to be perfect from day 1. Having meetings year after year with no improved InChI will sooner or later sow doubt in the minds of those financially supporting the project. I recently had a conversation with the IUPAC InChI subcommittee chair regarding the matter of examining the many InChI working groups and dropping or abolishing the ones for which there has never been any formal plans (just an idea that a topic should be addressed) and changing the make-up of those leaders and/or members are no longer participating in any meaningful way. The result of the conversation was complete agreement. The next step will be for the subcommittee chair and secretary to "clean house".

Chemical mixture composition (MInChI)

Leah McEwan has done a superb job in both leading the working group and actually getting a final set of specifications produced and delivered. Her project update report is attached to this report. There are two parts that needed to be programmed:
1. How to create the MInChI from the mixture input information
2. Handling of the input format

Chair: Leah McEwan
Members:
Gerd Blanke, StructurePendium Technologies
Alex Clark, Collaborative Drug Discovery
John Duffus, Edinburgh Centre for Toxicology
Richard Hartshorn, University of Canterbury
Chris Jakober, University of California

John LaRue, MilliporeSigma
Andrey Yerin, ACD

Isotopologues

The project is working on a deposition approach for NMR data from stable isotope-resolved metabolomics experiments. They have figured out how to generate isotope-representative InChI associated with possible NMR spectral features of metabolites. They are now trying to improve the process of generating these isotope-representation InChI representing partial isotopomers within a software package called isotopic enumerator.

Once the proposed improvements to InChI are implemented, they plan to expand the isotopic enumerator to handle isotopologue-representative InChI.
Chairman: Hunter Moseley
Members:
Philippe Rocca-Serra
Reza Salek
Masanori Arita
Emma Schymanski

Infographics

The Infographic is live on the InChI Trust website: https://www.inchi-trust.org/inchi-post/inchi-infographic/ , announced via Twitter: https://twitter.com/InChI_Trust/status/1065275928455118848. At Springer Nature, they are in the process of setting up a special website celebrating IYPT 2019 and IUPAC 100, and the infographic will be part of this. It is to go live will be around the first of January 2019.

As this effort appears complete it will no longer be included in future reports.

Positional Isomers

While considerable technical interest in positional isomers has developed in the past, no one is willing to take the lead for this area. The current members of this working group is in limbo are:

Christoph Steinbeck, Egon Willihagen, John May, Steffen Neumann, Steve Stein, Roger Sayle, Evan Bolton, Oliver Fiehn

At this point in time it would seem best to merge all these variable structures (Markush, positional isomers, and so on) into one working group. This should be able to happen with the current plans for the working groups to meet in Cambridge UK in February 2019.

Resolver

No further progress report has been submitted since my last report, which referred to what Marcus Sitzmann reported at the March 2016 meeting at EBI/Hixton.

This is a working group/project that is likely to be ended.

Polymers

With release of version 1.05 a limited area of polymer chemistry can now be handled by the InChI algorithm. A number of issues were found after release 1.05 and Igor continues to work on these matters.

As a result of feedback from the community Igor has added some extensions and has done a redesign. More regarding this can be found in Igor's 27 page report which was submitted to the Trust for the February 2019 Board meeting.

Reactions

Under the leadership and programming direction of Gerd Blanke this project has moved ahead very nicely. The RInChI 1.00 release was finalized in March 2017. Response has been very positive.
The working group is looking into possible modifications/enhancements in 3 areas:
The next release of the Biovia software packages Draw, Direct and Pipeline Pilot (release 2019, to be released in December 2018) includes RInChI. Therefore Biovia/Draw is the first drawing package providing direct access to RInChI. We are talking to other vendors to include RInChI to their software packages as well.
The RInChI group has started this summer to prepare the next release. Major issues we would like to address are

- Main level
    - Workarounds for stereochemistry and tautomer restrictions
        - Standard InChIs are always calculated based on absolute stereochemistry, racemates cannot be handled by standard InChIs.
        - More and more tautomers are represented by the same standard InChI (See results of Marc Nicklaus group). Tautomerisation reactions provide identical educts and products if you use standard InChIs.
    - Additional input and output formats (currently restricted to RXN/RD file format)
        - InChI with reaction roles
        - Under discussion: Reaction SMILES (depending on additional InChI converter)
        - Under discussion: UDM format of Pistoia Alliance
        - Under discussion: Standardized way to identify equilibrium reactions
            - RXN/RD and reaction smiles only handle forward reactions A -> B
    - Address failing reactions
    - If available for InChI: Make use of positional isomers and Markush representations for RInChI (questionable for next release)
    - Technical issues
        - Adaption to latest InChI version 1.05
        - Enhancements for command line tool
        - Programming issues
            - Thread safe libraries

        - Working MAC version
- Auxiliary level
    - Reaction mapping (MapAuxInfo)
    - Big data analysis methods
        - Reaction properties (ProcAuxInfo)
        - Class code layer for reaction similarity clustering and pathway optimization, InfoChem tool
        - Transform layer for pathway optimization, Reaxys tool (no feedback since meeting in Boston)

Time plan:
In February we would like to discuss those issues in the InChI meeting that depend on InChI as such like the representation of stereoisomers and tautomers within RInChI.
For the August meeting in San Diego we plan to represent the final list of requirements for the next RInChI release.

Chair: Gerd Blanke, StructurePendium
Members:

David Nicolaides	Biovia, Cambridge, UK
Günter Grethe	Retired, San Diego
Hans Kraut	InfoChem GmbH, Munich
Jan Holst Jensen	Biochemfusion AsP, Copenhagen
Jonathan M. Goodman	University of Cambridge, UK

009-043-2-800 Standard InChI-based Representation of Chemical Reactions
http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2009-043-2-800

Markush

It would seem most likely that the issues with Markush structures will be part of the variability working group issues to be resolved. This project will no longer be included in future reports.

Organometallics

Building sufficient momentum within the InChI community to overcome differences of opinion about how best to proceed towards revisions of the standard that will reliably accommodate organometallics has proved somewhat challenging. At a Task Group session in Boston, they discussed motivations that might help mobilise the community to action. Points raised included the following:

- Fundamental to integrity and perception of InChI - reputational risk if left unaddressed
- Community don't appear to be beating down the door - but perhaps patiently waiting for the working group to deliver
- Potentially significant opportunities for application - needs something to be built to explore if this is the case

This led to a commitment from experts present at the Boston workshop to convene a small group to focus on some concrete proposals for organometallic InChI that could be considered for implementation. They have since received one proposal for consideration; this and other ideas will be discussed at the next Task Group session planned for Cambridge UK in February 2019.

Chair: Colin Batchelor
Members:
Ian Bruno
Heike Nau
Markus Sitzmann
Keith T. Taylor
Dmitrii Tchekhovskoi
Andrey Yerin

Inorganics

A decision on how to proceed with this awaits the outcome of the Organometallics work

Large molecules, biopolymers/Proteins/biological polymers/macromolecules/biomolecules etc.

Progress continues to be very slow. I have not had a report yet again from Keith Taylor .

2013-010-1-800: Implementation of InChI for chemically modified large biomolecules
http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2013-010-1-800

Chairman: Keith Taylor

Members: Gerd Blanke, Evan Bolton, Didier Chalon, Alex Drijver, Jan Jensen, Andrey Yerin, and Helen Berman

There has bene no communication from the working group and it would seem necessary to find someone willing to chair and be active in moving this area forward.

Tautomers

Under the leadership of Marc Nicklaus, NIH/NCI, InChI project #2012-023-2-800, "Redesign of Handling of Tautomerism for InChI V2" was approved for funding by IUPAC and work has been ongoing.

The working group is almost finished with collecting all the materials for all the new transforms: SMIRKS, stats of occurrence, how well current InChI recapitulates them, experimental literature supporting them, etc.. They are at ~65 transforms, which includes the 20 standard CACTVS

transforms. They are also about to update our Tautomerizer web tool (https://cactus.nci.nih.gov/tautomerizer/) along the lines suggested by Evan Bolton and Greg Landrum, to have a separate "explanation & evidence" page for each of the transforms in addition to the actual tool. Marc's working group members promised to then look at each of them to finally come to a group decision which ones should be included in InChI V2. As Marc stated - Let's see if this will remain just empty promises and InChI will become an INickChI in version 2..
2012-023-2-800: Redesign of Handling of Tautomerism for InChI V2
http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2012-023-2-800

Chairman: Marc Nicklaus

Members: Evan Bolton
Wolf-Dietrich Ihlenfeldt
Tyler Peryea
Igor Pletnev
Hinnerk Rey
Markus Sitzmann
Dmitrii Tchekhovskoi,
Greg Landrum
John Mayfield
Roger Sayle,
Gerd Blanke
Alex Clark
Bret Daniel
Devendra Dhaked
Hitesh Patel
Laura Guasch

Extended Stereochemistry

Evan Bolton is still thinking about what to do in the area of stereogenic centers such as cumulenes. This proposed issue will no longer be included in this report until an actual plan is proposed.

QR Codes

The InChI QR code consultation workshop IUPAC project was approved in June 2015. Richard Hartshorn is leading this project. This is the announcement for this project:

"The InChI Trust (http://www.inchi-trust.org/) is examining development of a QR code (2D bar code) version of the InChI. We wish to consult with industry/regulatory/academic sector users to identify and prioritize additional information that could/should be included in the QR code to enhance the value and commercial utility of the QR InChI. Possibilities to be evaluated and elaborated upon include: health/safety information (hazard code and/or safety data URL); catalog

code; batch number; inventory information; sample composition/purity. This project is complementary to another user-focused project that is developing InChI for states and mixtures." There has been no new developments in this area to report.
Chair: Richard Hartshorn,
Members:
Jonathan Goodman
Jeremy Frey

Education/Academic/Training

In July 2018 the InChI OER (Open Education Resources) working group received funding from IUPAC, project no. 2018-012-3-024 (https://iupac.org/projects/project-details/?project_nr=2018-012-3-024) to develop and maintain an OER component to the InChI Trust website (Resources Tab on landing page). The task group consists of 8 members, with Steve Wathan joining in December, 2018.

The primary mission of the OER task group is to bring about a greater awareness of InChI in the education community, while also facilitating its use and adoption across other communities. There are two facets to this endeavor; creating original educational material, and creating a resources that allows educators and scientists to share material with others, with the latter being the mission of the OER website (https://www.inchi-trust.org/oer/).

The following posters and oral presentations were given during this time, and the people who manned them are indicated.

SWRM 2018: InChI OER: Open Education Resource on use of the International Chemical Identifier, SW Regional ACS meeting, Little Rock, AR, Nov. 18, 2018 (Belford & Bucholtz, poster) ECRICE 2018: InChI Open Education Resource, Warsaw Poland, Sep. (Cuadros, poster and oral presentation) Fall 2018 ACS National Meeting, InChI Open Education Resource, CINF Poster session (Scalfani & Belford, poster) 2018 BCCE: InChI Open Education Resources, Notre Dame University, IN, July 20, 2018 (Belford and Bucholtz, poster)

Note: There were no IUPAC or InChI Trust funds use for any of the poster presentations to date.

Belford also created a manual on how to upload content to the OER website and the taskgroup seeks to populate the site during the Spring of 2019, with the goal of presenting it as an operational facet of the InChI Trust website during the IUPAC centennial in July. A copy of the draft manual is attached with this report.

Chairman: Robert Belford
Members:
Nathan Brown
Ehren Bucholtz
Jordi Cuadros
Tanya Gupta
Vincent Scalfani
Martin Walker

Steven Wathen

August 2018 – December 2018 activities

Meetings Attended; Talks/Posters Presented

A number of conference call meetings with Ray Boucher, Richard Kidd and Ian Bruno were held over the past six months to deal with issues that needed to be addressed between Board meetings. I met on a regular basis with members of NIH/NCBI, particularly Evan Bolton, to discuss InChI issues.
I attended the August 2018 Trust Board meeting in Boston., the August working group meetings, and August 2018 ACS meeting in Boston.
As what seemed to be that I was the oldest living graduate (of 1963) I gave an invited Keynote Lecture on InChI at Stony Brook University for the Stony Brook Chemistry Department, 60th Anniversary Celebration, October 2018.
I gave a poster presentation at the GDCh meeting in Mainz, Germany in November, Among the results of attending the meeting was an invitation to give a lecture on InChI at the Sloan-Kettering Institute in NYC in January 2019.
The Education working group has been active and there have been two presentations by their members:
September 3, 2018 ECRICE 2018 in Warsaw Poland poster presentation by Jordi Cuadros
November 9, 2018 ACS SWRM 2018 in Little Rock, AR, poster presentation by Bob Belford and Ehren Bucholtz.
Public RInChI presentations in 2018:

- Talk at the ChemAxon UGM in Budapest by Gerd Blanke, March 2018
- Publication: International chemical identifier for reactions (RInChI), Grethe et al. J Cheminform (2018) 10:22 (May 2018)
- Poster at ICCS, Noordwijkerhout, May 2018
- Talk at ACS Fall meeting by Jonathan Goodman, August 2018
- Talk at the Biovia community days in Brussels by David Nicolaides and Gerd Blanke, November 2018

Manuscripts

No new manuscripts were published in the past six months.

InChI Trust web site

The Trust web is up on the InChI Trust cloud server.

InChI Usage

Numerous publications now use InChI as part of their efforts in merging and analyzing database structures. Clearly InChI is being used on a very regular basis in many organizations and research projects and publications.

InChI Trust Videos - Access numbers/Views as noted below continue to increase slowly every year:

InChI & the Islands – 1,269 (12/18) , 1,208 (7/18), 960 (1/17); 804 (1/16); 728 (7/15); 526 views (7/14)

The Googlable InChIKey – 2,115 (12/18) 1,985 (7/18), 1,379 (1/17), 1,037 (1/16) ; 915 views (7/15), 597 views (7/14)

The Birth of the InChI – 1,848 (12/18), 1,791 (7/18), 1,365 (1/17), 1,084 (1/16), 984 views (7/15), 687 views (7/14)

What on earth is InChI? - 6,750 (12/18), 6,102 (7/18), 4,188 (1/17), 3,331 (1/16), 2,956 (7/15), 2486 views (12/14); 1977 views (7/14)

IUPAC InChI (Google lecture - 2008) - 978 (12/18). 950 (1/17); 946 (7/16); 931 (1/16); 922 views (7/15)

An Update on the Open Source InChI Project – 2007 Google lecture 1,785 (12/18)

Technical Issues

As mentioned, numerous times, and supported by the work that Igor does every month, the mechanism to discuss and resolve technical issues continues to work well, as evidenced by the activities from the community during the testing and release of version 1.05.

Most issues seem to be able to be resolved by email and phone calls, but face-to-face meetings are still very critical as there are some very strongly held opinions that do not get resolved by emails. My regular meetings with NIH (PubChem, NCI, and FDA) staff have been very useful.

As for the current work being undertaken by Igor Pletnev the current tasks are the update of InChI FAQ's and preparing bug-fix InChI Software release, so-called v. 1.051.

Sustainability

As mentioned in my two previous reports, in discussions with a number of people about the long-term future and direction of the InChI project no one seems to have any good ideas for long term sustainability – both in a technical and administrative/financial sense. Hence, I am repeating my previous comments which I hope will be part of the InChI Trust Board strategy session being held in Cambridge in February 2019 along with other InChI meetings, such as the working group meetings

The technical issue of how to maintain and expand the InChI algorithm appears to be easier to deal with. Having one programmer maintain and add to the algorithm, with additional pieces (such as RInChI) coming from another programmer seems to be working well. The SourceForge group of programmers who test and provide feedback has been working well. The idea of using GitHub to have people around the world offer additions to the algorithm seems sensible in principle, but owing to the nature of InChI being an international standard, there are complications. Who decides at IUPAC if more features are needed? Or does the community (whomever they are) decide?

As for administrative and financial matters, things are a bit more problematical. IUPAC has never had a project like this which requires ongoing work and support. That was the main reason the Trust was established some 10 years ago. While the Trust has seemed to be working well for the past decade the issue of ongoing support from the current 16 Members and Associates is less clear. Much of the financial support really comes via individuals within the 16 organizations who believe in the project. We have seen in the past few years when some of the "founding" members change jobs their replacements do not have the same interest and enthusiasm for InChI.

This is not a unique issue. For many years scientists who developed databases had both funding problems to maintain and add to their databases as well as not receiving credit within their institutions for their efforts as this work was not considered publishable research. Well-known databases, such as Beilstein, which had been around for over a century, disappeared when the German government decided to terminate support. The world has changed since I first started working in the area in the 1970s. I and a number of my colleagues worked for various Government agencies and were able to move forward, while I doubt this would have been the case had we been in an academic setting.

InChI could continue as a standalone activity if proper institutional, political, and financial support were available. InChI could be adopted by an established organization whose long-term goals and plans could include InChI. For example, the RSC, ACS, or EBI could be a possible long-term home. NIST, as the US standards agency and the organization that developed the InChI algorithm, would make sense as well, if the right office at NIST would want to do it. The last initial suggestion would be the NIH/NLM/NCBI PubChem, an organization which has the expertise and is a major user of InChI.

Plans for 2019

For the 2019 my current overall plans and goals are as follows:

1. Work to expand the current membership with two basic classes of members – Full and Associate as well as add to the number of Supporters. Continue to attend meetings and give talks on InChI where useful and appropriate.
2. Meet with J Cheminformatics to discuss possible new InChI manuscripts to be submitted for publication.
3. Attend ACS meetings in Orlando March/April 2019 and San Diego August 2018.
4. Attend the April 2019 BioIT meeting and present a poster talk on InChI.
5. Possibly give an InChI seminar for Steve Boyer/Google patent staff in the spring of 2019.
6. Attend and participate in sessions on InChI, InChI working groups, and related standards at the Orlando and San Diego meetings

7. Attend the IUPAC General Assembly and InChI meetings in Paris, July 2019.
8. Attend IUPAC and InChI and InChI Trust Board meetings in San Diego.
9. Meet with groups to discuss adoption and usage of InChI.
10. Present InChI lectures in Beijing and Shanghai in May and June 2019.Meet with officials of the Chinese Chemical Society regarding joining the InChI Trust
11. Attend the November 2019 GDCh meeting and have a poster or oral presentation on InChI.
    .

Steve Heller

Appendix 5

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, *CCDC rep.*	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, *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

Appendix 6

Publications since Basel (August 2018)

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.

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).
J. Capitolis, S. Delacroix, X. Frogneux, E. Medina, N. Rey, L. Tinat, S. Carenso, Précis de nomenclature en chimie inorganique (French translation of the Brief guide to the Nomenclature of Inorganic chemistry): Actual. Chim. No. 437, 12 - 17 (2019), which can be accessed via the following url:http://www.lactualitechimique.org/Precis-de-nomenclature-en-chimie-inorganique

Názvosloví anorganické chemie podle IUPAC: Doporučení IUPAC 2005, – česká verze, Jaromír Vinklárek, 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).

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

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