

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

***Approved minutes for Division Committee Meeting  
Basel, Switzerland, 13–14 August, 2018***

**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, and noting the presence of three former Presidents of the Division, as well as the current Secretary General of IUPAC. He described the house rules and arrangements for the course of the meeting.

**2. Attendance and apologies**

*Present:* Alan T. Hutton (President, ATH), Karl-Heinz Hellwich (Past-President, KHH), Risto S. Laitinen (Secretary, RSL), Michael A. Beckett (MAB), Edwin C. Constable (ECC), Ture Damhus (TD), Richard M. Hartshorn (RMH), Elisabeth Mansfield (EM), Gerry P. Moss (GPM), Michelle M. Rogers (MMR), Molly A. Strausbaugh (MAS), Clare Tovee (CT), Andrey Yerin (AY)

(see also Appendix 1)

*Apologies:* Fabio Aricò (FA), Maria Atanasova Petrova (MA), Neil Burford (NB), (JC), Ana Maria da Costa Ferreira (ACF), Safiye Erdem (SE), Rafał Kruszyński (RK), Robin Macaluso (RM), , Ladda Meesuk (LM), Ebbe Nordlander (EN), Amelia P. Rauter (APR), Erik Szabó (ES), Keith T. Taylor (KTT), Jiří Vohlídal (JV)

*Invited observer:* G. Jeffery Leigh (GJL)

*No replies:* József Nagy, Sangho Koo

**3. Introduction of attendees**

A short round of introductions was made. A new titular member, Prof. Edwin C. Constable and a new Associate Member, Dr. Clare Tovee, were attending the meeting of the Division Committee for the first time in this function.

KHH informed the meeting that the following persons had passed away during recent years: Peter A. S. Smith (CNOC, Chair 1987-1991), Robert F. T. Stepto (SPT), Thomas E. Sloan (CNIC), and Robert B. Fox (Task Group Member of Cyclic macromolecules project, SPT). Their memory was respected with a few moments of silence.

**4. Approval of agenda**

The agenda for the meeting (Appendix 2) was approved. It was noted that the International Year of the Periodic Table will be discussed as a part of Item 8.

## **5. Approval of minutes of meeting in Sao Paulo, 8–9 July 2017**

This item was postponed to the beginning of day two of the current meeting, when some modifications were suggested for the draft minutes of the Sao Paulo meeting. The minutes were duly approved as modified.

## **6. Matters arising**

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

## **7. IUPAC strategic plan**

ATH made a presentation on the strategic plan of IUPAC (see <https://iupac.org/who-we-are/strategic-plan/>). There was a brief discussion, during which TD suggested that Division VIII should express dissatisfaction with regard to the efficiency of the administration of IUPAC (office, webpage, etc). AY remarked that IUPAC should stick to common terminology to help non-native speakers to understand the webpage content. GPM stated that IUPAC should improve communication with other outside organizations, not just with the chemical community. RHM noted that IUPAC is a very large organization but there are only 4-5 persons in the Secretariat. They are doing their best within the available resources.

## **8. Information from IUPAC Secretary-General, Professor Richard Hartshorn, on IUPAC's vision and planning, particularly around IUPAC's Centenary Year in 2019**

RMH made a brief presentation on the challenges that faced IUPAC and made the following key points:

*Strategic Plan:* RMH was very pleased to see the IUPAC Strategic Plan being reviewed in the meeting, since it provides a structure to help us think about what we are doing. Key motivations include working to improve the financial and membership states of the Union – which will involve making a real effort to demonstrate the value of IUPAC to its various membership categories. A new system for determining national subscriptions is being developed. There is a push to involve more companies. One way we can demonstrate value is by reaching out to other organisations (e.g. OPCW, REACH, ISO) to tell them what we are doing that is relevant and to find out from them the kinds of things that they may need from IUPAC.

*Succession planning is vital for the health of IUPAC:* It is important to identify and mentor future leaders and to bring in new blood (e.g. through projects). Diversity is important – we need to identify good candidates and get them nominated for elections. We also need to look forward and identify critical skill sets (e.g. cheminformatics, big data, and other strategic directions).

*IUPAC100 is important:* IUPAC has its centenary anniversary in 2019 and this will be celebrated at the General Assembly and Congress in Paris over the period 7–12 July 2019. Other events connected to the celebration of IUPAC100 are the “Global Womens’ Breakfast” and the “Periodic Table of Younger Chemists”. There will be articles published on IUPAC achievements. It is, however, also important to look forward to the next 100 years.

*International Year of the Periodic Table:* IYPT will be opened at UNESCO in Paris in January 2019 and closed possibly in Japan in December. Most activities will be done at a national level.

*Discussion:* Some points were raised concerning IYPT and other matters:

TD: In making the Danish version of the Periodic Table by the Danish NAO, there were problems with the spelling of Danish element names, amongst other things. There were also problems with the IUPAC office in obtaining the editable IUPAC Periodic Table. More support from the Secretariat to NAOs is needed. The national versions of the Periodic Table should be made available on the IUPAC webpage.

GPM: Although IUPAC works in English, other nationalities need their own languages. Information on translations should be distributed widely.

ECC: The RSC journal Dalton Transactions will produce a special issue on the Periodic Table in 2019. Wikipedia is also well ahead in creating international Periodic Tables.

GJL: The problem is that there are various forms of Periodic Table and different people prefer different forms. They all might be useful in special circumstances. While the Periodic Table can have many forms, it must contain the correct formal information.

RMH: The approved Periodic Table is the IUPAC Periodic Table.

EM: Young chemists (< 40 years of age) must be nominated for the IUPAC "Periodic Table of Young Chemists". These people will be associated with specific elements.

GPM: Atomic weights are revised every second year. Many chemists are not aware that atomic weights change. A new set came out in June 2018. This information needs to be widely distributed.

## **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 (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 (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 Karl-Heinz Hellwich (the Division IV counterpart still unclear). Both KHH and JV are members of SPT, providing natural overlap. RMH noted that there is a need to have continuity. The overlap with SPT is so important that it would be good to have two contact persons. It was decided that Andrey Yerin will 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.** Karl-Heinz Hellwich is contact person for Division VII (no known Division VII counterpart).

**\*Action:** Contact relationships need to be reactivated. RSL will contact the Secretaries of the above-mentioned Divisions to confirm these decisions.

**ICTNS.** Ture Damhus is the representative of Division VIII on ICTNS. KHH reported that in the meeting of ICTNS with all Division Presidents in Sao Paulo, it was noted that all relevant persons and bodies should be reminded that every document must be distributed to all relevant Divisions before submission to ICTNS. GPM noted that his term on ICTNS ended at the end of 2017. As noted last year in Sao Paulo (see Item 7 in the DC minutes), there are still problems in the handling of the documents during the ICTNS phase, which have resulted in a number of errors and delays in publication. MAB remarked that, from experience, the publication and review processes are currently very confusing.

There are several problems about interactions with ICTNS. Project outputs have been submitted to ICTNS but not acted upon. Answers to emails have been unsatisfactory. Procedures have been changed but task groups have not been informed. After submission to ICTNS, the refereeing and public review processes are no longer carried out simultaneously. The document is submitted to PAC through Manuscript Central. It then goes through the refereeing procedure, and only after the modifications goes to public review. ICTNS review for Recommendations includes members of ICTNS and external reviewers. Technical Reports require ICTNS review but not external or public review. There was confusion with this new system, largely because of a lack of response to questions posed.

SPT has formulated instructions on how the submission process should work. These provide guidelines to Task Group Leaders. The document also gives guidance on how joint projects should be handled. SPT accepted the document in Cairns in June 2018 and it will be shared with Division VIII. ATH remarked that he is not keen on different Divisions having separate instructions – IUPAC should have a unified set of instructions that apply to all Divisions. KHH replied that there were different circumstances that apply to Divisions IV and VIII. ATH insisted that it should still be a document that applied to all Divisions.

**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. Clare Tovee will be nominated as a Division VIII representative on the InChI Subcommittee.

CPCDS is currently involved in the new website of IUPAC and in InChI. In a recent meeting CPCDS expressed interest in closer contacts with Division VIII. The contacts with the InChI Subcommittee also need to be intensified (AY and CT) as much of the InChI's work is directly related to Division VIII interests (see also Item 11.3).

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

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

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

**Wikipedia.** KHH reported that there have been no further contacts since last year (see Item 7 in Sao Paulo minutes). The editorial board of Wikipedia is an *ad hoc* group of people. Anybody can make modifications in Wikipedia articles, but often the work of specialists is ignored. The editorial boards have the means to block changes in certain parts of the text. ATH noted that the checking of information and contacting the editorial boards would constitute a project rather than a contact. ECC remarked that since the work is open-ended, a subcommittee would be more appropriate than a project.

**\*Action:** AY will survey how serious the problem is. If needed, a project or a subcommittee will be established.

**JCBN (Joint Commission on Biochemical Nomenclature).** GPM is the chairman of JCBN, TD and APR are Associate Members, and KHH was an *ex officio* member until the end of 2017 and continues as an AM in 2018. ATH is now the *ex officio* member.

**REACH (Registration, Evaluation, Authorization and Restriction of Chemicals).** This is the European Union's chemical control law. It came into force in 2007 and had phased in volume-based registration deadlines from 1 December 2010 – 30 May 2018. REACH registrations are submitted to the European Chemicals Agency (ECHA) (<https://echa.europa.eu/home>). As part of these registrations, all registrants are required to submit an IUPAC name for the substance and for all constituents of the substance for multi-constituent and UVCB substances (UVCB = Substance of Unknown or Variable composition, Complex reaction products or Biological materials). For many industrial compounds that fall into these categories, particularly UVCB, it is not possible to generate a chemical name according to IUPAC rules. As a result, industrial companies are required to generate their own chemical names and submit them as an IUPAC name in order to obtain a registration. A few examples are listed below:

Name	EC#	CAS #
Fatty acids, tall-oil, oligomeric reaction products with maleic anhydride and rosin, calcium magnesium zinc salts	500-451-8	160901-14-4
Reaction products of bis(4-methylpentan-2-yl)dithiophosphoric acid with phosphorus oxide, propylene oxide and amines, C12-14-alkyl (branched)	931-384-6	-

12-Hydroxy stearic acid and its oligomers esterified with branched and linear octadecanol	940-268-4	-
Saponification and oxidation product of carnauba wax with acidic sodium dichromate solution esterified with 1-methyl-1,3-propanediol and subsequent saponification with calcium dihydroxide	700-725-9	-
Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-nitro-, disodium salt, reaction products with 4-[(4-amino-1-naphthalenyl)azo]benzenesulfonic acid monosodium salt	215-403-9	1325-65-1
Benzenesulfonic acid, 4-amino-, diazotized, coupled with resorcinol, reaction products with formaldehyde	288-599-7	85828-72-4
Benzenesulfonic acid, para-, monoalkylation products with C14-C18 branched olefins (C15 rich) derived from propene oligomerization, calcium salt, overbased including distillates (petroleum), hydrotreated, solvent-refined, solvent-dewaxed, or catalytic dewaxed, light or heavy paraffinic C15-C50	701-205-4	-
Boron, (benzenemethanamine)trifluoro-, (T-4)-, reaction products with Bu glycidyl ether	270-821-9	68478-46-6
Iron, complexes with diazotized 5-amino-2-(phenylamino)benzenesulfonic acid monosodium salt coupled with 4-[(2-hydroxy-3,5-dinitrophenyl)azo]-1,3-benzenediol, diazotized 4-nitrobenzenamine and diazotized 3-aminobenzenesulfonic acid monosodium salt	276-464-5	72207-77-3
Reaction products of sodium glucoheptonate with iron sulfate and ammonium hydroxide	946-072-5	-
Acetic acid, oxo-, sodium salt, reaction products with cresol and ethylenediamine, iron sodium salts	283-041-9	84539-53-7

In many cases the name supplied by the company is not accepted by ECHA upon their review of the dossier, and they propose an alternative name. At that point the company has the option to accept the name or work with them to negotiate an alternative name that is acceptable to both parties. The names proposed by ECHA do not appear to follow any systematic nomenclature rules.

As an IUPAC name is required to submit a registration, we should have the ability to influence the nomenclature for these complex names. Therefore, we should pursue the following items:

- Draft a scoping project before the end of the year to determine scope of the challenges faced with UVCB nomenclature and how to proceed with addressing the identified issues.
- Identify contacts at ECHA to discuss nomenclature concerns.
- Identify task group members to work on a new UVCB nomenclature project.

- Contact the InChI Mixture Group to ensure we have representation on the group as they can contribute to the solution.

**\*Action:** An informal group comprising MMR, TD and some others should scope the seriousness of the problem and propose a solution.

**ACS Nomenclature Committee.** MMR and MAS are the contact persons.

KHH: A Division VIII representative used to be invited to attend the meetings of the ACS Nomenclature Committee, but there have not been any recent invitations.

MMR replied that the committee meets twice a year for half a day, but has accomplished very little in the last several years. A change in operations is being planned. There is a new strategic plan and is as follows:

Vision: Enabling a common language for chemistry

Mission: Educate, facilitate and advocate for the use of chemical representation that support universal understanding of chemistry.

Goal 1: Achieve a common language of chemistry by educating its practitioners

Goal 2: Facilitate the interaction of chemists to implement appropriate chemical representations

Goal 3: Advocate for the use of a common language of chemistry

The committee was introduced to the new strategic plan in Spring 2018, and project team were established around the goals. At the fall meeting the project team will meet for the first time to begin project work. Through this we hope to see greater engagement between the committee and IUPAC, INCI (International Nomenclature of Cosmetic Ingredients) and other nomenclature bodies.

**\*Action:** MMR and MAS will send a link to the material of the ACS Nomenclature Committee and RSL will distribute it as appropriate. The RSC Nomenclature Committee will also be contacted by RSL.

## **10. New committee portfolios (Project Manager and Web Manager)**

ATH informed the Division Committee that, as immediate Past-President, KHH would be best placed to adopt the position of Project Manager, and that he has agreed to take on this portfolio. Since Division VIII has at any given time either a Vice-President or a Past-President with the duties of the Vice-President, the general principle in future would be that the Past-President the Vice-President will alternately hold the position of Project Manager.

Clare Tovee agreed to take on the portfolio of Web Manager for Division VIII. This would involve updating and posting items on the Division's webpage. Lynn Soby from the IUPAC Secretariat would provide training by webinar in due course.

## **11. Updates on Division VIII projects**

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

KHH reported that the alignment project was initiated at the end of 2017 (see Item 8.24 of Sao Paulo minutes). This project recognizes that the rules defining the seniority and order of writing of substituents and ligands may differ in substitutive and additive nomenclature, and also in some cases be not clearly defined, in particular if the name of the group is modified in multiple ways. The objectives of this project are to standardize and rationalize the writing of chemical names as much as is possible.

The task group held a three-day meeting in London in November 2017 at which the use of various modifications in substitutive nomenclature (e.g. kappa terms, isotopic modifications) was clarified. The meeting concluded that, once the seniority order of the various modification types was established, alphanumeric ordering should be used in the name, where appropriate. However, the specifics in many cases were left for future deliberations. The second meeting was held in Basel on 10 August 2018. Some open questions were resolved (e.g. the use of kappa in the context of borane and metallacycle nomenclature). The summary minutes of the November meeting were revised (see Appendix 3). It is intended that a report will be written for *Chemistry International*.

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

The task group met in February 2018 in Cambridge. This project is a continuation of previous projects. The project is moving forward slowly.

*11.3. IUPAC International Chemical Identifier (InChI) projects*

A report by Steve Heller together with the list of current InChI projects is presented in Appendix 4. AY reported that there will be a discussion at the ACS National Meeting in Washington, DC, over the period 16-18 August, concerning all aspects of InChI (the InChI Trust will meet during the last day).

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

AY reported that all principles and procedures are already developed and the project is now in the stage of prototype tool. The details can be found at the project page and progress tab:

[https://iupac.org/projects/project-details/?project\\_nr=2015-025-4-800](https://iupac.org/projects/project-details/?project_nr=2015-025-4-800)

*11.3.2. Identifying International Chemical Identifier (InChI) Enhancements – QR codes and Industry Application (2015-019-2-800, Richard Hartshorn)*

A journal article describing the InChI QR code standard is in preparation.

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

The question is whether there are any extensions to InChI needed to accommodate large biomolecules. InChI will have a small workshop in this connection at the ACS National Meeting.



*11.3.4. Handling of Inorganic Compounds for InChI V2 (2012-046-2-800, Richard Hartshorn and Hinnerk Rey)*

RMH reported that this project has not really been started. See also Item 11.3.6.

*11.3.5. Redesign of Handling of Tautomerism for InChI V2 (2012-023-2-800, Marc Nicklaus)*

AY reported that there is no information about the progress of the project.

*11.3.6. InChI requirements for Representation of Organometallic and Coordination Compound Structures (2009-040-2-800, Colin Batchelor)*

AY noted that there had been no recent progress. It had been decided earlier that InChI should also be used to describe  $\eta$ -bonding situations. The question is to scope what should be included, and how InChI would cope with metal–ligand bonds.

*11.4. 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)*

There is an extensive list of errata which has been compiled by GPM. More comments and errors in the Blue Book had been reported during the past year. The task group had met in Basel. That meeting also discussed the project dealing with the assignment of hydro prefixes (see Item 11.11) and some issues were also resolved relating to stereochemistry. It was decided that all errors that have been reported but not yet published should be processed and made public. Comments and corrections can still be sent to [bluebook@iupac.org](mailto:bluebook@iupac.org).

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

EM reported that during the past year the task group had considered chirality and added a section on chemical functionalization of the nanotubes. A new document will be distributed. The project is nearly finished.

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

KHH reported that the hyphenation project had made slow progress. In Sao Paulo the document revised by Jan Reedijk was considered. A meeting in September 2017 of KHH with de Gruyter was concerned with errors in end-of-line hyphenation (see Item 17). The publisher's typesetting software needs rules on how to employ end-of-line hyphenation that can be easily applied by non-specialists in chemical nomenclature. The task group had met in Basel to discuss the latest version of the document.

GJL: In the book "*Principles of Chemical Nomenclature*", a character ► [character code 25BA from Unicode (hex) in MS Word], which was not part of the name, was used to indicate the line-break. This usage has not been applied in other publications. KHH remarked that it needs to be a symbol that is readily available.

ECC noted that there is also a problem in breaking formulae between the lines, since use of the hyphen could change the meaning. KHH remarked that this document did not treat formulae.

Discussion ensued as to whether there should be a project to consider the hyphenation of formulae. ATH noted that there is not enough material to have an independent project on formulae and the same task group should consider this matter. RMH remarked that formulae should not have end-of-line hyphenation problems, because they are shorter and there are plenty of enclosing marks to divide the formula at the end of the line. After some debate it was concluded that whilst this document does not treat formulae *per se*, the principles of the proposed rules for names should also apply to end-of-line hyphenations for formulae and a short section should be included in the current document that comments on this matter and recommends what to do in the case of formulae.

*11.7. 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 joint project based of Division II in which Division VIII also has an interest. There is no new information, but the project should be close to publication. CT noted that there was a publication this year, which might be related to this project [C. Bonneau, M. O’Keeffe, D. M. Proserpio, V. A. Blatov, S. R. Batten, S. A. Bourne, M. S. Lah, J.-G. Eon, S. T. Hyde, S. B. Wiggan, L. Öhrström, Deconstruction of Crystalline Networks into Underlying Nets: Relevance for Terminology Guidelines and Crystallographic Databases, *Cryst. Growth Des.* **18**(6), 3411–3418 (2018)].

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

There had been a short meeting in Basel. The project has been waiting for resolution of various kappa issues being considered by the Alignment project. Now that some decisions had been made, further progress will be possible. AY noted that there had been confusion in the use of locants, while others reported that some errors of this kind had been corrected at the meeting. The next phase is to consider charged species.

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

MAB reported good progress during the last year. The Alignment meeting in November resolved open issues and enabled the continuation of the project. Submission to ICTNS took place in February 2018. Public review will end at the end of 2018. When the document was submitted, there were two versions: a clean version and the highlighted (commented) version. This caused some confusion, but now the submission contains only the clean version. The process of submission to ICTNS and PAC in connection with the public review is very complicated. It needs clarification and simplification.

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

There are two goals for the project: revising and integrating carbohydrate conjugates. This task has turned out to be more extensive than was originally anticipated. A second extension of the project was applied for and has been approved. A considerable part of the nomenclature section was revised at a meeting in Cambridge in the spring of 2018. There is still work to be done on the glycoinformatics part. TD noted that glycoinformatics researchers are discussing how to define a carbohydrate. There is a need to increase the interaction of synthetic chemists with informatics.

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

There was a meeting of the task group in Basel prior to the Division Committee meeting. The main purpose of the document is to compare the four systems in use. The document has to be consistent with the Blue Book, and the Blue Book needs to be modified. There are several unresolved questions: selection of the full set of locants, and whether they can be omitted in special cases. It is also sometimes not obvious which nomenclature system is being used. The progress of the project depends on the handling of the errata part of indicated hydrogen involved in Blue Book revision. Once that has been resolved, the document can be processed further.

*11.12. Terminology and nomenclature of inorganic and coordination polymers (2011-035-1-800, Richard Jones); abbreviated as "TINCOPS"*

TD reported that there had been no progress over the last year. The project aim is to update an old IUPAC recommendation from the 1980s. It is worth noting that the old document was reprinted, unchanged, in the 2000 Red Book (Chapter II-7). New drawings need to be made, and the kappa convention needs to be taken into account. Lars Öhrström is the acting chair while the actual chairman is ill.

*11.13. 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)*

The Inorganic Brief Guide has been published. KHH reported that the task group on the Organic Brief Guide had met in Sao Paulo and the text and formula changes were decided on that occasion. A new version was created earlier this year. The task group also met in Basel and the manuscript is expected to be submitted to ICTNS soon. There is a need to provide both the four-page brochure version and a ca. 12-page version in PAC format.

*11.14. Glossary of small molecules of biological interest (2009-022-2-800, Karl-Heinz Hellwich)*

The task group had a meeting at the end of May. This project has a complex history. The original objective was to provide nomenclature rules for molecules of biological interest that are not covered in other documents due to the lack of suitable compound classes. There is a need for a simple document only dealing with some important small molecules of biological interest, rather than for the production of the full-scale database. The chairman, Marcus Ennis, who had taken this project over

from Dick Cammack, had resigned from JCBN earlier in the year and Gareth Owen has been appointed to replace him.

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

KHH reported that a document had been submitted to ICTNS. This document had recently been published electronically in *PAC* after several rounds of proofs. If no further errors are found, the document will appear also in print in due course. AY inquired as to why the document contains Appendix 2 and 18 pages of InChIs. KHH reported that this was to satisfy the request of one referee.

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

TD reported that this project had evolved to concern only the kappa convention. Kappa formalism is used to specify the connection between donor atoms and the central atoms. There are the following aspects to consider: (i) Can donor atoms always be given locants? (ii) The central atoms can relatively easily be formulated, but can their locants be separated from the kappa symbol? (iii) Where will the kappa term be placed?

In the Alignment task group meeting in London (see Item 11.1), the priority of the kappa term was considered in relation to other modifications. There are subgroups looking at these different questions. When some sample structures have been considered, a new manuscript can be written for the kappa document. As far as the original title of the project is concerned, little progress has been made. Possibly the project should be renamed. KHH noted that the name of the project and the titles of the documents it produces do not need to be the same.

**\*Action:** ATH will inquire whether a change in the project name is feasible.

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

GPM reported that this is an old project, which had recently been resurrected. It is now seeing progress. A text document and separate files for each table have been combined into a single file, which is being reviewed by JCBN.

*11.18. Polymer projects (with Division IV)*

There are several projects with Division IV–Division VIII partnership. KHH made the following reports:

*11.18.1. Graphical Representation of Polymer Structures (2017-039-2-800, Karl-Heinz Hellwich)*

This is a new extension of an old project. A first meeting was held in Cairns in June 2018. There are several documents existing of different ages. The current intention is to homogenize the graphical representation and combine everything into one document. The task is expected to be completed in October 2018.

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

The task group had met in Sao Paulo. This project is about conjugated macromolecules. The basic idea is that the names of the components remain unchanged, and there is a linking term to describe the structure. During the Cairns meeting, details of the linkings were discussed. A need for simpler examples was considered. KHH will design systematic names. This is important not just with polymers but also large conjugated pharmaceuticals where a protein is link to another cytoactive molecule by a linker (usually a shortish molecule). The protein is selective for say cancerous cells and the cytoactive molecule will selectively kill the cancerous cell.

*11.18.3. Structure-based Nomenclature for Regular Linear, Star, Comb and Brush Polymers (2013-031-3-800, Jiazhong Chen)*

After a task group meeting in Sao Paulo a new draft was prepared and was discussed in Cairns in June 2018. It was noticed after the meeting that several older comments had not been taken in to account. This is now being rectified. There is a follow-up project, but it is on hold until this project is finished.

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

A document is ready but unfortunately contains erroneous citations that need to be corrected. The manuscript had been on hold for two years. In Cairns in June 2018 some critical points were discussed and other minor corrections were made. The document is close to the review process.

*11.18.5. 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)*

There had been a task group meeting in Sao Paulo without the presence of the task group chair. A telephone meeting was held in April 2018, after which the manuscript was submitted to ICTNS. The document was originally intended to be placed only on the IUPAC webpage, but after the Sao Paulo meeting it was considered suitable also for submission to *PAC*.

*11.18.6. 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)*

This project has a modified title. It was published in *PAC* in November 2017.

*11.18.7. Guidelines for abbreviating polymer names (2006-004-1-400, He)*

There is nothing new to report.

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

This document has been completed and has been through the public review. After approval new errors were found. It was submitted for publication in June 2018.

*11.18.9. Nomenclature and terminology for lactic acid-based polymers (2012-042-1-400, 2014-033-1-400, Michel Vert)*

The document was submitted to ICTNS last year after the Sao Paulo General Assembly and was then reviewed by Division VIII in November 2017. There were very few comments, but a long list of corrections was supplied by KHH. A completely new draft was prepared, which again needed to be corrected. Ten versions of the document had been prepared up until March and it was re-sent to ICTNS in April 2018.

*[Secretary's note: Not on original agenda. Added during the discussions]*

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

The Solid-State Terminology Project members met at the IUPAC GA in Brazil. The group agreed to propose and define a bonding tetrahedron. This tetrahedron is an extension of the well-known van Arkel triangle, which describes bonding by its three corners being related to ionic, covalent and metallic bonding. The tetrahedron will add a fourth corner to the triangle with van der Waals bonding. We have assigned at least two project group members to define and identify literature examples for each of the four corners (and all edges).

During the Brazil meeting, project members met with members of the Interdivisional Subcommittee of Materials Chemistry and identified their website as a likely place to host the educational materials that we produce as part of this project.

We were well on our way to writing this paper, but there has been a delay because of my pregnancy and birth of a child (in March). Now that I will be back to work in August and September, the project will resume. The group may meet once again in Spring 2019 to make further advances on the paper. We have been working well through e-mails and Skype up to this point and will continue communicating in this manner.

*[Secretary's note: This written report from RM was received immediately after the meeting.]*

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

GPM reported that this project should have been finished by November 2017, but there was no information as to whether it had been concluded. According to KHH, it was reported last year that a document had been published, but the manuscript had not gone through ICTNS.

**\*Action:** ATH will write to the President of Division III to inquire about the current status of this project.

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

KHH reported that this project was said to have been cancelled and replaced by a new project. There is no information about the new project. The Gold Book is expected to have a new platform.

**\*Action:** ATH will enquire about the current status from Leah McEwen.

*11.22. Rules for Abbreviating Protecting Groups (2011-044-1-300, Margaret Brimble)*

This is a project in which RMH, APR and GPM have been involved. KHH reported that there is a published document (2014), which contains many nomenclature errors. This work still needs to be completed, but nothing had happened during the last year. There is budget left, so there could be a meeting to revise the document.

**\*Action:** ATH will write to APR to enquire about current status.

## **12. Future projects/activities**

*12.1. International Organization for Standardization (ISO) liaison: Nanoparticles project.*

There is already an established project working on the nomenclature of carbon nanotubes (see Item 11.5). There should also be a project on nanoparticle nomenclature. A scoping meeting was held in London in 2015. ECC has prepared a project proposal for clusters, but a task group needs to be formed. Richard Hartshorn, his colleague Vladimir Golovko, Ebbe Nordlander and Alison Smith could be candidates.

**\*Action:** The draft project proposal will be circulated and ATH will coordinate liaison with ISO to produce a nanoparticle nomenclature project.

*12.2. 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 are already active. The Division Committee could be a managing body. There could be scoping project, but the discussion and planning could be done by email. A draft of the contents should be prepared.

**\*Action:** RSL will prepare a first draft of the contents and distribute it to the whole Division.

*12.3. Central webpage for all IUPAC Recommendations/publications.*

This would be an interdivisional task and the webpage would also provide guidance to authors when preparing Recommendations and Technical Reports. The resultant database should be searchable. GPM noted that the current IUPAC website does not contain all IUPAC

Recommendations. The content ends when de Gruyter took over (2017). This project was concluded not to be of a high priority. The project should, however, be kept in mind in the background. TD and GPM noted that the website managed by GPM is easily searchable and much easier to use than the IUPAC webpage.

**\*Action:** Clare Tovee will discuss the possibilities with Fabienne Meyers.

- 12.4. *UVCB (Substance of Unknown or Variable composition, Complex reaction products or Biological materials) 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 introduced the general problematics and outlined the need for having proper nomenclature for industrial chemicals (see also Item 9). ATH remarked that it was possibly too soon to propose a project. MMR noted that probably industry might not be too interested in nomenclature and companies will not change their names unless required to by official bodies.

**\*Action:** MMR will draft a scoping project and make a contact with the InChI Mixtures Task Group.

- 12.5. *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.).*

TD described the problem of having too many different categories of names (“approved”, “systematic”, “provisional”, etc.). This is not a project but should be an activity of Division VIII to simplify and rationalize the hierarchy. RMH remarked that there has to be a distinction between nomenclature and terminology – as it is, there is often confusion. While normally concepts such as “accepted”, etc. are understood to apply only to names, they should also apply to terminology. This needs to be discussed with ICTNS. TD suggested that the only terms we need to use are “recommended” and “not recommended”. However, KHH noted that if the name is clearly wrong, there must be a way to state that it is wrong. There is also a need to be able to express the notion that a name is not acceptable.

**\*Action:** An internal report should be written, possibly also an article in *CI*.

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

Division VIII and the Committee for Chemistry Education (CCE) have contributed equally to this project, which has now been approved and can be listed as a Division project.

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

The Organization for the Prohibition of Chemical Weapons (OPCW) and IUPAC are embarking on a mutual venture of cooperation in which all IUPAC Divisions will participate. It is a short term project, lasting no more than a year. There will be a meeting in November 2018 in Den Haag in The Netherlands and Division VIII should send a representative to this meeting. RHM explained that



IUPAC and OPCW had signed a memorandum of cooperation. The role of OPCW is changing from active detection of the use of chemical weapons to educating people so that chemical weaponry does not appear again. New ways for cooperation between IUPAC and OPCW should be explored. An IUPAC delegation will attend the annual meeting of OPCW in Den Haag in November 2018. All IUPAC Divisions are committed to send a representative to the meeting. OPCW is closely tied with the UN and the delegates to the meeting will consist largely of diplomats. IUPAC should assist in setting the standards on various forms of chemical representations. The Division VIII representative would be expected to be involved in interactions with diplomats and other people. GPM noted that proper IUPAC names are needed for existing and new chemical warfare compounds. There will also be OPCW people attending Division Committee meetings and participating in the GA in Paris in 2019. MMR noted that there is a need for education to promote the understanding of what constitutes a chemical weapon, and which substances might be used in them.

There was a brief discussion of suitable persons to represent Division VIII (ATH, ECC, GJL, GPM were mentioned as possibilities), but no final decision was taken.

#### *12.8. Other projects*

*12.8.1.* GJL mooted that a *Revision of the Principles book* should be initiated. Such a revision should take into account the needs of school teachers and students. GJL noted that in addition to this revision, there is a need for a text book. ECC remarked that an App could possibly be more useful than a book. RMH and MMR observed that the Brief Guides could easily be converted to use on mobile phones. The App should have a capability that when a formula is photographed, the App can provide the name. KHH reminded the meeting that the work of Division VIII is to provide content, not the form, which is the job of IT people. ATH noted that there is an obvious need for collaboration with CPCDS. This is also related to discussions with CCE (see Item 9.14.4 of Sao Paulo minutes).

**\*Action:** ATH, GJL and AY will look into this and possibly form a project. GJL will scope the need for an actual revision of the Principles book.

#### *12.8.2. Unicode for chemistry.*

CPCDS thought in Sao Paulo that creation of a Unicode for chemistry would be a good idea, but nothing has happened since then.

#### *12.8.3. Electronic representation of polymers*

AY suggested that THIS should be a separate project from graphical representation. It would be a joint Division VIII–SPT project. The general idea would be to give guidance on how to present polymers, provide the tools of presentation, and give instructions on how to draw structures. Software developers also need to be educated. There is a good list of people who would like to be involved. AY would be the Task Group leader. KHH noted that such a project should run together with the project on graphical representation, but it will have to wait for results from that project.

### 13. IUPAC nomenclature consultancy/naming service/contact addresses for users, etc.

KHH reported that there is a contact form on the IUPAC webpage offering the possibility to inquire about nomenclature problems, but it is not clear how such requests should be handled.

**\*Action:** ATH will inquire from Lynn Soby or Fabienne Meyers about the processes in place for these kinds of requests and how they should be answered.

### 14. Membership matters

#### 14.1. Status of Division VIII Committee membership

The current Division VIII roster is shown in Appendix 7. 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 possibility of including subcommittee chairs on the Division roster was discussed and approved.

**\*Action:** Subcommittee chairs will be included on the Division VIII roster as *ex officio* committee members. ATH will contact LME.

#### 14.2. Division VIII representatives on other IUPAC bodies

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

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

#### 14.3. Division VIII Advisory Subcommittee

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 approved minutes of the Sao Paulo Division Committee meeting, and inquire 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.

ATH proposed that there should be some kind of prestigious emeritus membership of the Division for people who have strongly contributed in the past, and that such a scheme should be incorporated in the Division Rules (see Item 16). ECC noted that Division VII already has an elegant system of emeritus membership.

**\*Action:** ATH will draft a proposal for criteria to appoint deserving individuals to such emeritus membership (*cf.* the IUPAC Fellowship).

#### 14.4. Nominating Committee

KHH explained that the Nominating Committee should contain four members: two from the Division Committee and two from outside IUPAC. Their task is to nominate ten candidates for possible election as Titular Members in the Division elections next April/May.

*[Secretary's note: It was subsequently established that the Nominating Committee should comprise five members, two from the Division Committee and three from outside IUPAC.]*

**\*Action:** ATH will prepare a proposal for the composition of the Nominating Committee.

### 15. JCBN Terms of Reference, Composition and Terms of Office

KHH reported on the history and development of the organization of the Joint Commission on Biochemical Nomenclature (JCBN). In 2001 all Commissions (including JCBN) were dissolved. Since JCBN is an inter-union Commission, its new status was negotiated (see Appendix 5). There are issues concerning the terms of reference and terms of office (see Appendix 6), in particular concerning the duration of the terms of service. While IUPAC has a maximum of 12 years of membership service, JCBN defines it differently, since continuity is an important issue. This also has reference to the consultancy function of the enzyme group. It must be noted that any change in the terms of reference, composition, or the terms of office must be approved by both the IUPAC Council and by IUBMB.

GPM described the funding of JCBN. The Secretary is funded by IUPAC, the Chair by IUBMB, and the Titular Members by the two Unions. KHH remarked that all commissions must be approved by the Council every two years. It was concluded that the Division will be happy to see the revised terms of reference. All aspects need to be negotiated with IUBMB.

**\*Action:** KHH and GPM will prepare the application for new terms of reference including terms of office of JCBN, but the application must be signed by the Chair of JCBN. The Division Committee will consider these terms of reference at a later stage.

## 16. Formulation of Division Rules

The Secretary General of IUPAC has requested that each Division should formulate a set of Division Rules (or Operating Procedures). ATH remarked that Divisions I and VII already have these, and Division III has a shorter set of rules. RMH noted that if there are existing old rules for Division VIII, they will be distributed to all Division presidents. ATH suggested that there could be one set of rules for all Divisions, not separate rules for each individual Division. RMH noted that different Divisions have different duties and composition and therefore individual rules may be easier to administer. Such a document would be a valuable guide for incoming Division Officers and Committee Members.

**\*Action:** ATH will investigate the existence of earlier Division VIII rules, consult currently available rules of other Divisions, and compile a draft set of new rules for Division VIII.

## 17. A report from a meeting with De Gruyter Production

KHH reported on his visit to the De Gruyter editorial/production offices. The meeting was mainly concerned with hyphenation. However, other problems were raised concerning document formats, such as italicization and some other automatic formatting features. Whereas various items of format were correct in the submitted manuscripts, there were errors introduced at De Gruyter in the proofing stage. The outcome of the meeting was that the staff at De Gruyter are keen to cooperate in fixing the problems. It is imperative that the content and formatting of our manuscripts are not changed, since these are the responsibility of the authors and critical in defining the rules for naming compounds. De Gruyter agreed that symbols should not have been italicized automatically, in particular as this was not done consistently. Cross-referencing was also a problem (mainly due to automatic page numbering). It was concluded that the interaction with De Gruyter should be continued and developed.

## 18. Publicity

### 18.1. Division VIII (and related) publications since the 2017 Division Committee meeting

The publications involving Division VIII since the Sao Paulo General Assembly in July 2017 are presented in Appendix 8. Recent publications involving nomenclature are also listed on the website managed by GPM. The German translation of Source-based Nomenclature has been published in *Angew. Chem.* (see Appendix 8)

*[Secretary's note: KHH reported after the meeting that in the context of the book "Comprehensive Glossary of Terms Used in Toxicology", the appendix with the systematic names for toxic compounds had been thoroughly corrected by KHH and reviewed by GPM and TD for ICTNS. KHH also reported that the "Red Book" had been translated into Czech and reviewed by JV with a few comments by AY and KHH. The book is now with the publishers, with publication expected in September 2018.]*

### 18.2. *IUPAC–IUBMB nomenclature website*

GPM reported that the information of the usage of the website, as provided in previous years, is no longer available.

### 18.3. *IUPAC website*

ATH noted that while there have been serious efforts to improve the IUPAC website, it is still not user friendly. KHH remarked that in improving the website, new errors have been introduced and important items are sometimes hidden deep in the hierarchy. RMH promised that the issues of search functions, structure, and relationships with the databases will be looked at carefully. The current emphasis is rather to serve the outside community than IUPAC itself.

GPM noted that a related problem involves *PAC*. It is difficult to browse issues, since there is no scroll bar and therefore it is not possible to see all issues. KHH remarked that the *PAC* website seems to change every 1–2 weeks, which is very inconvenient for users.

**\*Action:** All Division Committee members should test the websites and communicate their experiences to RSL, who will compile a list and send it to ATH, who will contact the IUPAC Secretariat. KHH will contact the Chair of the Editorial Board of *PAC*.

## 19. **Reports from other IUPAC bodies**

### 19.1. *ICTNS*

Interactions with ICTNS had been discussed earlier in the meeting (see Item 9). The Division VIII representative on ICTNS, TD, commented further that a number of things did not work well, and that old reviews were not visible. KHH said that there had been a short meeting in Sao Paulo, where it was made clear that documents sent to ICTNS should be seen by all relevant Divisions before submission to ICTNS.

### 19.2. *JCBN*

GPM reported that one major document had been published: Flavonoids. The phosphorus project (2006-019-1-800) had been revived (see Item 11.17). The project on small molecules of biological interest (2009-022-2-800) will also be re-activated (see Item 11.14). The enzyme project is continuing to provide a useful service. There is a new development in enzyme nomenclature: it has been decided to establish the seventh category of EC-7 transferases. TD noted that, according to the bylaws, Division VIII should provide guidance in enzyme nomenclature. TD was currently going through the glossary to supply and correct IUPAC names. GPM reported that a brief guide to enzyme nomenclature was proposed as a project that would be compiled by the enzyme sub-committee. Although it did not require money it would probably have to become an IUPAC project if it is to be published in *PAC* (and elsewhere).

### 19.3. *CCE*

**\*Action:** RM will be asked to send a report on the recent activities in the Committee for Chemistry Education.

## **20. Any other business**

KHH announced that there were copies of the Inorganic Brief Guide and the Beilstein Stereochemical Descriptors booklet available at the meeting for distribution. ATH noted that claim forms will be sent out with instructions on how to divide the expenses from different sources. He also informed the meeting that there would be a 30-day time limit to submit the claims. There was no further business.

## **21. Dates and venue for next meeting**

KHH noted that the Division Committee would meet on the second and third days of the General Assembly in Paris, i.e. on 6 and 7 July 2019. RMH described the problems in scheduling the upcoming General Assembly timetable of the meetings because of the centenary celebrations of IUPAC coupled with the events connected with the International Year of the Periodic Table.

A possible venue for the off-year meeting in 2020 was discussed. Possible places were Canada, Finland, South Africa (there is the International Conference on Chemistry Education in Cape Town over the period 13–17 July 2020), as well as the USA. Further discussion on this was deferred to the Division Committee meeting in Paris in July 2019.

## **22. Adjournment**

ATH thanked the participants, the previous Presidents, ECC for local arrangements, and the Division Secretary for capturing the minutes. A group photograph was taken (see Appendix 1). The meeting was adjourned at 12h30.

**Attendees of the Division Committee meeting of Division VIII in Basel on 13.-14.8.2018**



Sitting: Alan T. Hutton (President, left), Risto S. Laitinen (Secretary, right)

Standing from left to right: Karl-Heinz Hellwich (Past-President), Andrey Yerin, Gerry P. Moss, Michael A. Beckett, Jeffery Leigh, Richard M. Hartshorn, Molly A. Straughbaugh, Michelle M. Rogers, Clare Tovee, Ture Damhus, Edwin C. Constable. Not in the photo: Elisabeth Mansfield

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

***Draft agenda for Division Committee Meeting  
Basel, Switzerland, 13–14 August, 2018***

- 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 Sao Paulo, 8–9 July 2017**
- 6. Matters arising**
- 7. IUPAC strategic plan**
- 8. Information from IUPAC Secretary-General, Professor Richard Hartshorn, on IUPAC's vision and planning, particularly around IUPAC's Centenary Year in 2019**
- 9. Interactions between Division VIII and other (IUPAC) bodies in relation to documents and projects involving chemical nomenclature.**
- 10. New committee portfolios (Project Manager and Web Manager)**
- 11. Updates on Division VIII projects**
  - 11.1. Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature (2017-033-1-800, Karl-Heinz Hellwich)*
  - 11.2. Graphical representation standards for chemical reaction diagrams (2003-045-3-800/2012-033-1-800/2017-036-2-800, Keith T. Taylor)*
  - 11.3. IUPAC International Chemical Identifier (InChI) projects*
    - 11.3.1. InChI extension for mixture composition (2015-025-4-800, Leah McEwen)*
    - 11.3.2. Identifying International Chemical Identifier (InChI) Enhancements – QR codes and Industry Application (2015-019-2-800, Richard Hartshorn)*
    - 11.3.3. Implementation of InChI for chemically modified large biomolecules (2013-010-1-800, Keith Taylor)*



- 11.3.4. Handling of Inorganic Compounds for InChI V2 (2012-046-2-800, Richard Hartshorn and Hinnerk Rey)*
- 11.3.5. Redesign of Handling of Tautomerism for InChI V2 (2012-023-2-800, Marc Nicklaus)*
- 11.3.6. InChI requirements for Representation of Organometallic and Coordination Compound Structures (2009-040-2-800)*
- 11.4. 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)*
- 11.5. Nomenclature of carbon nanotubes and related substances (2013-056-1-800, Elisabeth Mansfield)*
- 11.6. End-of-line hyphenation of systematic chemical names (2014-003-2-800, Albert Dijkstra)*
- 11.7. Terminology guidelines and database issues for topology representations in coordination networks, metal-organic frameworks and other crystalline materials (2014-001-2-200, Lars Öhrström)*
- 11.8. Nomenclature for metallacycles containing transition metals (2013-030-1-800, Alan Hutton)*
- 11.9. Nomenclature for polyhedral boranes and related compounds (2012-045-1-800, Michael Beckett)*
- 11.10. Revision and extension of IUPAC recommendations on carbohydrate nomenclature (2012-039-2-800, 2015-035-2-800, 2017-026-1-800 Johannes Vliegenhart )*
- 11.11. A comparison of assignment of hydro prefixes, added and indicated hydrogens in IUPAC, CAS and Beilstein nomenclature systems (2012-037-1-800, Andrey Yerin)*
- 11.12. Terminology and nomenclature of inorganic and coordination polymers (2011-035-1-800, Richard Jones); for short TINCOPS*
- 11.13. 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)*
- 11.14. Glossary of small molecules of biological interest (2009-022-2-800)*
- 11.15. Nomenclature of flavonoids (2009-018-2-800, Amelia Rauter)*
- 11.16. Preferred names for inorganic compounds (2006-038-1-800, Ture Damhus)*
- 11.17. Nomenclature of phosphorus-containing compounds of biochemical importance (2006-019-1-800, Gerard Moss)*
- 11.18. Polymer projects (with Division IV)*

- 11.18.1. Graphical Representation of Polymer Structures (2017-039-2-800, Karl-Heinz Hellwich)*
- 11.18.2. Nomenclature for polymeric carriers bearing chemical entities with specific activities and names (2014-034-2-400, Michel Vert)*
- 11.18.3. Structure-based Nomenclature for Regular Linear, Star, Comb and Brush Polymers (2013-031-3-800, Jiazhong Chen)*
- 11.18.4. Definitions and notations relating to stereochemical aspects in polymer science (2009-047-1-400, Karl-Heinz Hellwich and Graeme Moad)*
- 11.18.5. 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)*
- 11.18.6. 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)*
- 11.18.7. Guidelines for abbreviating polymer names (2006-004-1-400)*
- 11.18.8. Terminology and structure-based nomenclature of dendritic and hyperbranched polymers (2001-081-1-800, Alain Fradet and Jaroslav Kahovec)*
- 11.19. Survey of Definitions and Use of Common Solid-State Chemistry terminology (2015-053-1-200, Robin Macaluso)*
- 11.20. Nomenclature of Homodetic Cyclic Peptides Produced from Ribosomal Precursors (2015-003-2-300, Martin Reaney)*
- 11.21. IUPAC Color Book Data Management (proposal 2013-052-1, Kinnan)*
- 11.22. Rules for Abbreviating Protecting Group (2011-044-1-300, Margaret Brimble)*

## **12. Future projects/activities**

- 12.1. International Standards Organization (ISO) liaison. Nanoparticles projects (c.f. item 11.5).*
- 12.2. New edition of Nomenclature of Inorganic Chemistry, the 'Red Book'.*
- 12.3. Central webpage for all IUPAC recommendations/publications.*
- 12.4. 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.*
- 12.5. Proliferating IUPAC terminology to denote that names are (maybe) acceptable (recommended, retained, preferred, alternatively used, sometimes used, widely used, ...) or not acceptable (not recommended, (strongly) discouraged, not included in these recommendations, deprecated, ...) or to characterise them otherwise (common, traditional, trivial, ...).*
- 12.6. InChI Open Education Resource (OER) (proposal 2018-012-2, Robert Belford)*

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

12.8. *Other projects.*

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

**14. Membership matters**

14.1. *Status of Division VIII Committee membership*

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

14.3. *Division VIII Advisory Subcommittee*

**15. JCBN Terms of Reference, Composition and Terms of Office**

**16. Formulation of Division Rules**

**17. A report from a meeting with De Gruyter Production**

**18. Publicity**

18.1. *Division VIII (and related) publications since the 2017 Division Committee meeting*

18.2. *IUPAC-IUBMB nomenclature website*

18.3. *IUPAC website*

**19. Reports from other IUPAC bodies**

19.1. *ICTNS*

19.2. *JCBN*

19.3. *CCE*

**20. Any other business**

**21. Dates and venue for next meeting**

**22. Adjournment**

**Alignment of principles for specifying ligands and substituent groups across various areas of nomenclature.  
Summary minutes**

**Meeting:** Department of Chemistry, Kings College London, November 20-22, 2017.

**Present:** Karl-Heinz Hellwich (chair), Michael Beckett, Edwin Constable, Ture Damhus, Richard Hartshorn, Alan Hutton, Risto Laitinen (secretary), Gerry Moss, Ebbe Nordlander, Andrey Yerin

**Apology:** Warren Powell

**Introduction**

The names of chemical compounds are most commonly formulated by use of either substitutive nomenclature, which is applied for organic and many non-metallic main group compounds, or additive nomenclature, which is used for naming coordination complexes and other inorganic species. In many cases, the rules defining the seniority and order of writing of substituents and ligands may differ in substitutive and additive nomenclature, and also in some cases be not clearly defined, in particular if the name of the group is modified in multiple ways. The objectives of this project are to standardize and rationalize the writing of chemical names as much as is possible. The kappa term has been used within additive nomenclature to identify the site of coordination and this discussion was initiated from a consideration of the hierarchical positioning of this descriptor and the possible consequences for the structure of the substitutive name of the ligand. The goal is to reach consensus in following open questions:

- the grouping of substituents or ligands with different kinds of modifications
- the alphabetical order of substituents or ligands with different kinds of modifications
- the positioning of locants for substituents and ligands in chemical names
- the positioning and grouping of kappa terms in chemical names
  
- total description of the enclosing marks including nesting order, when appropriate

The following summarizes the main discussions and decisions. Some important directions for future nomenclature development were also discussed.

**Ordering/grouping of modified substituents and ligands**

***General***

The ordering is affected by two different considerations: the seniority of the atoms and groups of atoms and the order of writing the name based on alphanumeric considerations. The latter principle was explored in detail during this meeting.

The alphanumeric ordering is based on the principle "nothing comes before something". This implies that the unmodified name of the substituent or ligand is cited first and is followed by the modified substituents and ligands, provided they are otherwise identical. Atom numbering and locants are independent of alphanumeric ordering and are based on the seniority principles.

### Examples

1. The name 'butyl' is cited before 'sec-butyl', which is cited before 'tert-butyl'.

In substitutive nomenclature, the choice of the parent is based on seniority principles. In additive nomenclature, the central atoms are also ordered using seniority principles. Once the parent name has been decided, the modifications are listed according to the following priority ordering (the character '>' implies the item on the left side has a higher priority):

*lambda > substituents > isotopic modification > kappa > stereodescriptors* (see Note <sup>1</sup>)

Lambda,  $\lambda$  is a part of the parent name and has higher priority than other modifications. On the other hand, kappa,  $\kappa$  does not change seniority. However, kappa represents the coordination to a central atom and that connection might lead to a choice being made between two parents (e.g. which of two heterocyclic rings is chosen as a parent in a hypodentate ligand) (see Note <sup>2</sup>).

### Isotopically modified compounds

An isotopically modified compound has been defined in the Blue Book (P-81.5) as a compound, which "has a macroscopic composition such that the isotopic ratio of nuclides for at least one element deviates measurably from that occurring in nature". There are two types of isotopically modified compounds. An

---

Note <sup>1</sup>. Another priority sequence was proposed in the discussion after the meeting: *lambda > isotopes > stereo > substitution > kappa/eta*. This relies on the principle that the ligand is named first and it is only then established, how and where it is connected to the central atom. During the meeting it was noted that there are cases where kappa could determine configurational descriptions and this was used to justify placing kappa off the bottom of the priority list. It was proposed that the connectivity issues must be resolved before configuration can be determined, and since kappa describes connectivity, it must be considered before configuration. Each substituent has its own parent and can have its own modifications.

Note <sup>2</sup>. While alphanumeric citation follows the principle "nothing before something", the order based on seniority is exactly opposite. The parent name is based on the highest seniority and is cited last.

isotopically substituted compound has a composition such that essentially all the molecules of the compound have only the indicated nuclide at each designated position. For all other positions, the absence of nuclide indication means that the nuclide composition is the natural one.

An isotopically labelled compound has been defined in the Blue Book (P-83) as “a mixture of an isotopically unmodified compound with one or more analogous isotopically substituted compound(s). Although an isotopically labelled compound is really a mixture as far as chemical identity is concerned (in the same way as is an unmodified compound), for nomenclature purposes, such mixtures are called 'isotopically labelled' compounds.”

Isotopic modification involves in principle all areas of chemical nomenclature. Isotopic substitution is indicated in parenthesis and isotopic labelling in square brackets. The order of citation should follow the rule. The isotopically modified groups of atoms have higher seniority than corresponding unmodified groups of atoms.

The order of citation is the following:

higher number of substitutions > higher mass number > alphabetic order of nuclide symbols (Note <sup>3</sup>)

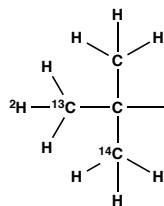
#### Example

2. Order of citation in the name, should more than one group occur in the same compound:

- A methyl
- B (*R* or *S*)-(<sup>13</sup>C, <sup>2</sup>H<sub>1</sub>, <sup>3</sup>H<sub>1</sub>)methyl
- C (<sup>13</sup>C, <sup>2</sup>H<sub>1</sub>)methyl
- D (<sup>14</sup>C)methyl
- E (<sup>13</sup>C)methyl
- F (<sup>12</sup>C)methyl-methyl-(<sup>13</sup>C, <sup>2</sup>H<sub>1</sub>)methyl-(<sup>14</sup>C)methyl-

---

Note <sup>3</sup>. It has been defined in the Blue Book (P-82.3.1) that “when isotopes of different elements are present as nuclides in an isotopically substituted compound, their symbols are arranged in alphabetical order if they are at the same place in the name.”



Citation order: A before B before C before D before E before F

In this example, the alphanumeric order of the citation for various methyl groups refer only to complete isotopic substitution. The relative citation order of the isotopically substituted and labelled compounds in the name need to be decided at a later stage. It was not considered in the London meeting.

If there are other modifications, their order of citations needs also to be taken into account.

#### Example

#### 3. Order of citation in the name (needs to be decided)

- A  $[^2\text{H}]$ sulfanyl
- B  $[^{34}\text{S}]$ sulfanyl
- C  $[^2\text{H}, ^{34}\text{S}]$ sulfanyl
- D  $\lambda^4$ -sulfanyl
- E  $[^{34}\text{S}]-\lambda^4$ -sulfanyl
- F  $[^2\text{H}_3]-\lambda^4$ -sulfanyl (Notes <sup>4</sup> and <sup>5</sup>)

In case of ligands in a coordination compound, the  $\kappa$  term to indicate the ligating atom could be added, as appropriate, to any of names in Example 3 without affecting the order of citation.

---

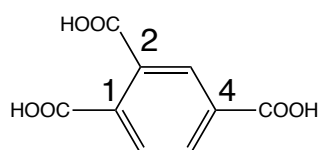
Note <sup>4</sup>. Note that  $\lambda$  is a part of the parent name and has higher seniority to other modifications. In alphanumeric ordering it is therefore cited just before the parent name.

Note <sup>5</sup>. The alphanumeric order of citation of  $[^2\text{H}](^{34}\text{S})$ sulfanyl or  $(^{34}\text{S})[^2\text{H}]$ sulfanyl needs to be discussed later.

Examples 4 and 5 illustrate the priority order of identical functional groups that contain different modifications, in this only case isotopic modification. The labelled group is cited last in the name, the parent name can also change.

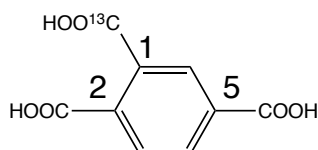
### Examples

4.



benzene-1,2,4-tricarboxylic acid

5.



2,5-dicarboxy-[<sup>13</sup>C]benzoic acid (Note <sup>6</sup>)

There are several open points, which follow from the considerations above but which were left for future deliberations:

- Does the modified unit or the unmodified group have seniority (see also BB, P-82.5.2)? It will affect the parent name and the numbering of atoms (Note <sup>7</sup>).
- If a modified group is senior to the unmodified group, it must be valid regardless of the relative locants.
- Once seniority and therefore the atomic numbering has been decided, everything follows by use of the principle nothing comes before something.
- If two atoms or group of atoms are modified similarly, they are treated as two modifications (Note <sup>8</sup>).

Note <sup>6</sup>. This name was considered ambiguous, since it is not clear if <sup>13</sup>C is part of benzene or the carboxy group. It was suggested that one labelled carboxy group is senior to two unlabelled (Blue Book P-83.1.2.2) and the name is therefore 2,5-dicarboxy[carboxy-<sup>13</sup>C]benzoic acid. A suggested alternative name would be 2,5- dicarboxybenzene[<sup>13</sup>C]carboxylic acid. In addition to modifications like isotopic substitution, the description of coordination would benefit from use of benzenecarboxylate derived names.

Note <sup>7</sup>. The relative seniority of the coordinating group with respect to other modifications should take into account that, where possible, it is better to have the coordinating group closer to the central atom in the full name.

Note <sup>8</sup>. The name for H<sub>2</sub><sup>15</sup>NCH<sub>2</sub>CH<sub>2</sub><sup>15</sup>NH<sub>2</sub> could equally well be ethane-1-[<sup>15</sup>N]amine-2-[<sup>15</sup>N]amine, or ethane-1,2-[<sup>15</sup>N<sub>2</sub>]diamine. If the nitrogen atoms are labelled differently, the long form of the name must be used. The choice is left for future discussions.



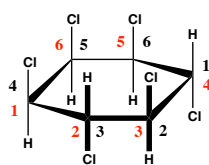
In the future revisions of the Blue and Red Books, there must be a section discussing the seniorities of different kinds.

### ***Modification by stereodescriptors***

In the name, the stereodescriptors come first and are therefore determined last, after every other aspect of the name had been determined. One aspect to consider involved the relative order of citation of stereodescriptors. The Blue Book does not address this issue.

#### *Example*

6.



$(1R,2r,3S,4R,5r,6S) R > r > S > s$

$(1R,2S,3r,4R,5S,6s) R > S > r > s$

Should upper-case symbols be preferred to lower-case. If so, stereogenic centers would be preferred to pseudostereogenic centers.

The rules need to be designed both for seniority, which affects the numbering, and for alphabetic ordering of the name components. Given an arbitrary choice, the priority could go either way and should also be considered in terms of the simplest way to program naming software.

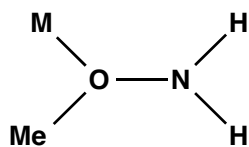
Since pseudochirality can appear only if real chirality is present, it was felt that real should take precedence before pseudo. Therefore, the priority between the upper and lower case will be  $R > S > r > s$ . However, this requires further discussion and exploration, so no firm decision was made on the matter.

### ***Position and grouping of kappa terms***

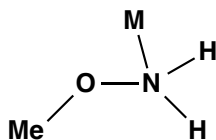
The organic ligand in a coordination complex is generally named using substitutive nomenclature. The seniority of the central metal atom is defined by the use of element sequence (BB Appendix 1, RB Table VI), which determines the numbering of atoms. The metal atoms are also cited in the order of the element sequence. The ligating atom should be indicated by  $\kappa$ , which appears immediately after the name of the relevant ligand component.

*Examples*

7.

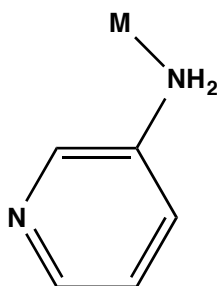


(*O*-methyl hydroxylamine- $\kappa O$ )

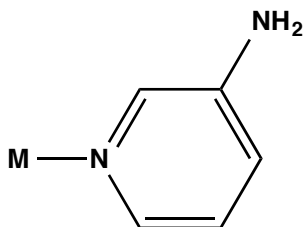


(*O*-methyl hydroxylamine- $\kappa N$ )

8.



pyridin-3-amine- $\kappa N$

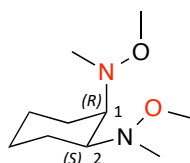


pyridin- $\kappa N$ -3-amine

The identification and numbering of central atoms is currently under discussion. The numbering of the metal atoms may result in a different set of locants from those of the ligands. Multiplicative prefixes may be used, when there are two identical parts.

*Example*

9. Free ligand

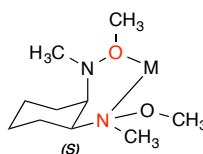
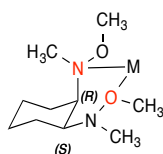


(1*R*,2*S*)-1,2-bis[methoxy(methyl)amino]cyclohexane

or

(1*R*,2*S*)-*N*<sup>1</sup>,*N*<sup>2</sup>-dimethoxy-*N*<sup>1</sup>,*N*<sup>2</sup>-dimethylcyclohexane-1,2-diamine

Coordinated ligand



If stereochemistry is not taken into account, both modes of coordination will lead to complex with a same ligand name:

1-[methoxy(methyl)amino-κ*N*]-2-[methoxy-κ*O*-(methyl)amino]cyclohexane

However, since the configurations of the atoms 1 and 2 in the uncoordinated ligand do not change because of the two different modes of coordination, the two stereoisomers have different stereochemical descriptors:

(1*R*,2*S*)-*N*<sup>1</sup>-[methoxy-*N*<sup>2</sup>-(methoxy-κ*O*)-*N*<sup>1</sup>,*N*<sup>2</sup>-dimethylcyclohexane-1,2-diamine-κ*N*<sup>1</sup>]copper

and

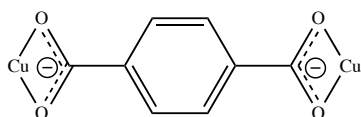
(2*R*,1*S*)-*N*<sup>2</sup>-[methoxy-*N*<sup>1</sup>-(methoxy-κ*O*)-*N*<sup>1</sup>,*N*<sup>2</sup>-dimethylcyclohexane-1,2-diamine-κ*N*<sup>2</sup>]copper

The seniority is not clearly established in the situation, where, for instance, the molecule contains two carboxylate groups, one which is isotopically modified and the other is coordinated. If two ligands are not exactly identical, they cannot be named using multiplicative prefixes. The difference may in different ligation or in modification, which further removed from the central atom. In some cases, it is still an unresolved problem, how number and indicate locants to donor atoms of the ligand, when it is named using substitutive

nomenclature. One possibility would be the use of nodal numbering or the application of InChI, but this will require further development.

### Examples

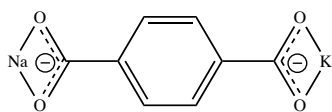
10.



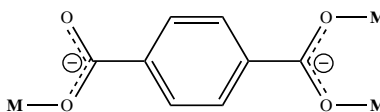
$\mu$ -benzene-1,4-dicarboxylato-( $1\kappa^2O^1,O^1,2\kappa^2O^4,O^4$ )dicopper,

Note that the locants for the ligating oxygen atoms are based on the numbering of the carbon atoms in the benzene ring. This is not a satisfactory method to indicate the donor atoms and further development work is needed (Note <sup>9</sup>).

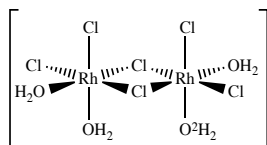
11.



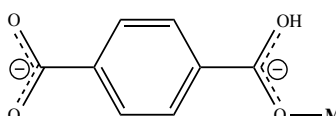
12.



13.



14.



There are also cases, where the concepts  $\kappa$  and  $\mu$  overlap. This dilemma needs to be dealt with in the coming recommendation concerning the use of  $\kappa$  in coordination complexes. The next revision of the kappa document will consider and modify, as needed, all existing examples in the current draft.

Note <sup>9</sup>. This is exactly the unsolved problem in the kappa document. In some EDTA-based examples it is necessary to go even more bonds away from the coordinating atom/group to find a locant that might be used. It can be unclear as to where in the name one has to go to “use” the locant to attach the group. The current conclusion is that one cannot use multiplicative nomenclature when the multiplied groups are connected to different central atoms. Another solution would be to apply the nodal numbering scheme or InChI.

### ***The effect of the use of $\mu$ and $\eta$ in the ordering***

There are no clear rules about the effect of the use of  $\mu$  and  $\eta$  on the ordering of the names of the ligands. While the problem of  $\eta$  was not considered, that of  $\mu$  was discussed in length. While not specifically stated in the Red Book, it has been commonly understood that the bridging ligands should be cited first. This is in contradiction to the alphanumeric ordering of ligands and the principle of 'nothing before something'. According to Red Book, the  $\mu$  ligands could come before the name of an otherwise similar terminal ligand, but otherwise the ligands are cited in alphanumeric order. This matter will have to be reconsidered during the future Red Book revision.

### **Consequences for borane and metallacycle documents**

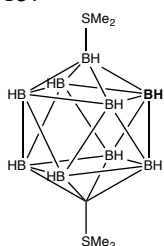
Both the borane and metallacycle documents need to be checked for consistency with the ranking decisions made in this meeting. Some examples were discussed in case of both documents and modifications were suggested. The revised manuscripts will be produced in the near future.

It seems to be evident that in these systems the substitutive and additive nomenclature need to be jointly applied in the same name. This, of course, is a completely new development in chemical nomenclature. The only exception to date has been the use of organic naming practise in naming organic ligands, the name of which is then combined into an additive name of the complex (Note <sup>10</sup>).

One important question to solve is the use of a locant in connection with the kappa term. This question has a clear correlation also to the situation with boranes. It has been suggested that as a compromise the locant of the ligand could be replicated in the kappa term.

### ***Examples***

15.



1,10-bis(dimethylsulfane- $\kappa$ S)-1,10-didehydro-*closo*-decaborane(10)

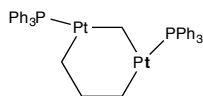
or

1-(dimethylsulfane-1 $\kappa$ S)-10-(dimethylsulfane-10 $\kappa$ S)-1,10-didehydro-*closo*-decaborane(10)

---

Note <sup>10</sup>. Red Book (Chapter IR-9) specifies that organic ligands should be named following the Blue Book, but the rigorous following of the substitutive principles and the inherent numbering might not always be possible and requires further work.

16.

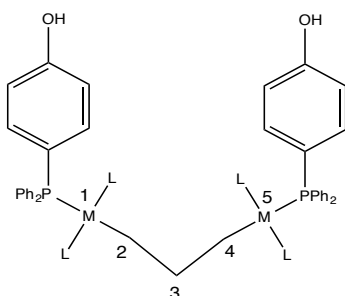


1,3-bis(triphenylphosphane- $\kappa P$ )...

or

1-(triphenylphosphane-1 $\kappa P$ )-3-(triphenylphosphane-3 $\kappa P$ )...

17.



1,5-bis[4-(diphenylphosphanyl- $\kappa P$ )phenol]...

or

1-[4-(diphenylphosphanyl-1 $\kappa P$ )phenol]-5-[4-(diphenylphosphanyl-5 $\kappa P$ )phenol]...

A sufficiently clear rule could be formulated in which a complete set of instructions is given with full replication of the locant in the kappa term. In simple cases this usage could be simplified and the replication is not needed. Examples need to be formulated to see if this approach leads to problems.

### Numerical prefixes

The common recommendation to date has been that the numerical prefixes di-, tri-, tetra-, etc. are used in simple cases and the parallel set of prefixes bis()-, tris()-, tetrakis()- are used in more complicated cases, which could lead to ambiguities. There has, however, not been a clear rule and the current Blue Book allows the use of di(), tri(), etc.. The following examples clarify the problem.

#### Example

18.

$\text{TlI}_3$

$\text{Tl}(\text{I}_3)$

thallium tris(iodide)

thallium triiodide

- |     |                 |                           |
|-----|-----------------|---------------------------|
| 19. | $\text{BaI}_2$  | $\text{Ba}(\text{I}_3)_2$ |
|     | barium diiodide | barium bis(triiodide)     |

Several examples in the metallacycle document were discussed. They will be brought in line with the decisions in this meeting.

### Enclosing marks and their role in the context of modifications

The use of enclosing marks has to be harmonized. While normal nesting order should be encouraged, there are instances, where enclosing marks have specific meanings and may result in two consecutive similar kinds of enclosing marks.

Enclosing marks need to be used, when modifying the ligand with lambda or isotopic labelling or substitution. The ligands will also be written inside the enclosing marks together with the kappa terms. The open question concerns the inclusion of the locant with the kappa term of the ligand inside the enclosing marks. Another consequence is that monoatomic ligands should also be written inside enclosing marks. It also has an impact on the use of multiplicative prefixes. There will therefore be a need to revise the Red Book.

#### Examples

- |     |   |
|-----|---|
| 20. | Multiplicative prefixes: di(chlorido) or bis(chlorido)  |
| 21. | Lambda:                    4-( $\lambda^5$ -phosphanyl) ...<br>4-(1 $\lambda^5$ -diphosphan-1-yl) ...   |
| 22. | Kappa:                    ( $\mu$ -benzene-1,4-dicarboxylato-1 $\kappa^2$ O <sup>1</sup> ,O <sup>1</sup> ,2 $\kappa^2$ O <sup>4</sup> ,O <sup>4</sup> ) ... |
| 23. | Isotopic modification: 1,3-di( $^2\text{H}_1$ methyl) ...<br>3-([ $^2\text{H}_1$ ]methyl) ...<br>1,3-di([1- $^{13}\text{C}$ ]ethyl) ...                     |

The consistent use of enclosing marks needs further discussion both within the Division Committee and with the chemical community. This matter could be brought up in *Chemistry International*.

## Element sequence

The element sequence in the Red Book is defined using the so called 'snake table' (Table 6), and in the Blue Book it is defined in the list of Table in Appendix 1. While the order of the elements is the same, their application to the determination to seniority might be different in different cases. The problem was discussed in depth, but any decisions were deferred to a later date.

## Summary and outlook

There are several different considerations: the seniority and the order of writing the name based on alphanumeric considerations. In writing the name in alphanumeric order, the principle 'nothing before something' will be applied. This results in the following priority order:

*lambda > substituents > isotopic modification > kappa > stereodescriptors*

Lambda,  $\lambda$  is a part of the parent name and has higher priority than other modifications. On the other hand, kappa,  $\kappa$  does not change the writing order in the name. The effect of the descriptors  $\mu$  and  $\eta$  on the naming priorities require further consideration.

In isotopically modified compounds, the following priority order is retained

*higher number of substitutions > higher mass number > order of nuclide symbols*

The ligating atom should be indicated by  $\kappa$ , which appears immediately after the name of the relevant ligand fraction. If two otherwise identical ligands are not coordinated identically, multiplicative prefixes cannot be used. In some cases it is useful to replicate the locant given as a prefix in the kappa term. In simpler cases, there could be rules simplifying this approach.

The normal nesting order of the enclosing marks will not be followed in the cases, where enclosing marks carry specific information and can result in two consecutive enclosing marks of the same kind. The use of enclosing marks in different areas of nomenclature requires further exploration.

These considerations will affect the currently active projects:

- Preferred names for inorganic compounds (kappa document and central atom selection) (2006-038-1-800)
- Inorganic and coordination polymers (2011-035-1-800)
- Boron hydride nomenclature (2012-045-1-800)



- Metallacycles nomenclature (2013-030-1-800)
- Blue Book revision and extension (2015-052-1-800)

The future project on Red Book revision will also have to take these considerations into account.

The possibilities to report results in the current alignment project could involve, in addition to an internal report, also a communication in *Chemistry International* and/or a technical report or recommendation in *Pure and Applied Chemistry*. At this stage a communication in *CI* seems to be most worthwhile.

# **InChI Trust Project Director's Report**

**July 2018**

## **Summary:**

Since the December 2017 report there continues to be good progress 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 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. More organizations, databases, and publications continue to use the InChI algorithm. As part of the 100<sup>th</sup> anniversary of IUPAC the InChI project was asked to contribute an article to the IUPAC100 project, which was published in February 2018

## **Items covered in this report:**

Membership/Support  
InChI RFP/Contracts  
InChI development work  
IUPAC InChI subcommittee and working groups  
Meetings attended & Talks/ Posters given  
Manuscripts  
InChI Trust Web Site  
InChI Usage  
Technical Issues  
Sustainability  
Plans for 2018

## **Membership/Support:**

Summary

There were no new memberships since the last report. An initial interest and further email correspondence from the Chinese Chemical Society (CCS) is waiting for further decisions on their part.

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.

As of July 20, 2018

Existing Members and Associates: 16 (only 15 are listed on the web page)

Supporters: 47

Lastly, Chris Boehm, the new Elsevier member of the Trust Board has left Elsevier and will be replaced in due course.

## **InChI RFP/Contracts**

There have been no contract activities since the last report.

## **InChI Development 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. Gerd Blanke continues to work on the RInChI algorithm. An RFP for the MInChI programming is expected to be issued in the fall of 2018.

## **IUPAC InChI subcommittee & working groups**

### **InChI work Groups**

#### **Chemical mixture composition (MInChI)**

Leah McEwan has done a superb job is both leading the working group and actually getting a final set of specifications produced and delivered. Her project update report is attached as a Word file to this report: MInChI-report-3-18 as well as a file of 4 PowerPoint slides: MInChI-slides-3-18.

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

## Isotopologues

In January 2018 an isotopologues working group was established and is led by Hunter Mosley. Hunter is working with representatives from the major metabolomics repositories (Metabolomics Workbench and MetaboLights) to develop an unambiguous identification scheme for mass spectrometry and NMR spectral features corresponding to specific isotopologues and isotopomers of chemical entities in metabolic samples. InChI can handle most of the isotopomer-specification needs, except with respect to isotopologues, which are mass-equivalent sets of isotopomers. Considerable progress has been made with his working group and final specifications are expected before the end of 2018. A write up from the working group is attached to this report. Additional material from their Metabolomics Workshop session is expected by mid-August 2018.

Chairman: Hunter Moseley

Members: Emma Schymanski, Reza Salek, Philippe Roca-Serra, and Masanori Arita

## Infographics

In January 2018 Board member Steffen Pauly from Springer-Nature proposed that an infographic (<https://en.wikipedia.org/wiki/Infographic>) be developed for InChI. Steffen has been able to secure support from Springer-Nature to undertake this effort and a draft of the infographic has been distributed for comment and review, and approval at the August 2018 InChI Trust Board meeting in Boston. An initial version will be available on the Springer-Nature web site for further public and user comment.

## 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 in limbo are:

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

There is a discussion underway concerning a number of areas of chemistry in which variable positions are an integral requirement. For example, besides positional isomers there are organometallics, inorganics, and Markush. Most of these working groups have been meeting for long periods of time without a final resolution. This should be an agenda item for the August 2018 IUPAC InChI subcommittee working groups meetings as well for the InChI Trust Board meeting.

**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.

**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.

**Reactions** – Under the 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:

1. Technical enhancements like the adaption to InChI 1.05
2. Changes in the format to handle racemization, tautomerization, etc.

Additional input and output format (depending on InChI development)

3. New developments like generic reactions and an implementation of the procauxinfo (please remember the talk in Fulda by a process chemist from Cambridge University UK)

They report that the first issue can be handled pretty soon, the second one is more that we need to agree the formats, number three will take longer.

Lastly, Gerd and colleagues published a manuscript on RInChI in *J. Cheminformatics* in May 2018. (see section on manuscripts for details)

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](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2009-043-2-800)

Chairman: Gerd Blanke

Members:

Gunther Grethe, Colin Batchelor, Jonathan Goodman

Hans Kraut, Martin Schmidt, Keith Taylor

**Markush** – With no interest from the US and other patent offices, this project remains on indefinite hold, but the possibility of starting work on it (mentioned above) could be realized if there is sufficient interest and need and funding.

**Organometallics**- Colin Batchelor and his working group have held two meetings in 2017. These meetings have uncovered important disagreements between people who are familiar with the code as to the best way to proceed. The working group is looking into a mechanism for finding people to make a proper investigation into disconnection and normalization of coordination and organometallic structures, potentially using the CSD APIs as a source of structures.

**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 from Keith Taylor this time.

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](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

I expect a write up from this working group to be attached to this report before the Board meeting.

**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. There is nothing new report as of now.

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](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, Marcus Sitzmann, and Dmitrii Tchekhovskoi

**Extended Stereochemistry** - Evan Bolton is still thinking about what to do in the area of stereogenic centers such as cumulenes.

## **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.”

## Education/Academic/Training

Bob Belford (University of Arkansas at Little Rock) has agreed to lead an effort for educational and training materials, such as an InChI primer, to help educate and make using InChI easier. The initial effort began at the August 2017 InChI meeting at NIH. Bob is assembling a working group of academics to go forward with this idea. Bob has drafted a IUPAC project plan, “InChI OER (Open Education Resource)” and will submit it to IUPAC for funding in 2018. The initial site is available at:

<https://www.inchi-trust.org/oer/>.

They have developed a draft outline for the taxonomy as follows:

### 1. *InChI Algorithm and Description*

- a. *Algorithm*
- b. *Software*
  - i. *Toolkits*
  - ii. *Resolvers*

### 2. *InChI Application*

- a. *General*
- b. *Classification*
- c. *Indexing*
- d. *Database Linking and Maintenance*
- e. *Data Extraction and Mining*
- f. *Data Sharing*
- g. *Data Validation*
- h. *Descriptors*
- i. *Search*
- j. *Standardization*
- k. *Structure Identification*
- l. *Structure Enumeration*

### 3. *InChI Modification*

- a. *Reactions*
  - i. *RInChI*
- b. *Extensions*
  - i. *General*
  - ii. *Inorganics and Organometallics*
  - iii. *Macromolecules*
  - iv. *Mixtures*

### 4. *Audience*

- a. *Researcher*
- b. *College and Universities*

- i. Undergraduate
    - ii. Graduate
  - c. Primary and Secondary Schools
  - d. General Public

## 5. Curricular Material

- a. Course material
  - i. Organic Chemistry
  - ii. Inorganic Chemistry
  - iii. Biochemistry
  - iv. Cheminformatics
  - v. Physical Chemistry
  - vi. Medicinal
  - vii. Pharmaceutical
- b. Activity
  - i. Lecture material
  - ii. Laboratory material
  - iii. Quiz material
  - iv. Homework

## 6. Content Type

- a. Poster
- b. Presentation
  - i. slideshare
- c. Document
- d. Spreadsheet
  - i. smartspreadsheet
- e. Movie
  - i. YouTube
- f. Software
  - i. Application
  - ii. Script
- g. publication

## 7. File Type

- a. Powerpoint (ppt/pptx)
- b. Word Doc (doc/docx)
- c. Exel (xls/xlsx)
- e. Python
- e. R
- f. Matlab
- g. Google doc
- h. Google Sheet
- i. Libre Office Calc
- j. Mov
- k. Avi
- l. Mp4
- m. Pdf



Chairman: Robert Belford

Members: Vincent Scalfani, Jordi Cuadros , Tanya Gupta, Ehren Bucholtz, Bob Hanson, and Martin Walker.

## January 2018 – July 2018 activities

### Meetings Attended; Talks/Posters Presented

A number of conference call meetings with Ray Boucher, Richard Kidd, and Alan McNaught 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 January 2018 Trust Board meeting in London.

I attended the March 2018 ACS meeting in New Orleans.

I attended the BioIT meeting in May in Boston and presented an InChI poster, as well as meeting with Fabienne Meyers who is located in Boston

### Manuscripts

The InChI for IUPAC100 manuscript has been submitted: "IUPAC and InChI Provide a Common Language for Chemistry. Ray Boucher, Stephen Heller, Richard Kidd, Alan McNaught, and Igor Pletnev

1. Ray Boucher, Stephen Heller, Richard Kidd, Alan McNaught, and Igor Pletnev, What on Earth is InChI?, IUPAC 100 Stories, IUPAC 100th Anniversary web site, February 1, 2018, <https://iupac.org/100/stories/what-on-earth-is-inchi/>

2. International chemical identifier for reactions (RInChI),  
Guenter Grethe, Gerd Blanke, Hans Kraut and Jonathan M. Goodman  
Journal of Cheminformatics, 201810:22  
<https://doi.org/10.1186/s13321-018-0277-8>  
<https://jcheminf.springeropen.com/articles/10.1186/s13321-018-0277-8>

### 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 – 1,208 (7/18), 960 (1/17); 804 (1/16); 728 (7/15); 526 views (7/14)

The Googlable InChIKey – 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 – 1,791 (7/18), 1,365 (1/17), 1,084 (1/16), 984 views (7/15), 687 views (7/14)

What on earth is InChI? - 6,102 (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)– 975 (1/18). 950 (1/17); 946 (7/16); 931 (1/16); 922 views (7/15)

## Technical Issues

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 January 2018 report, 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 Boston in August 2018 along with other InChI 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 2018

For the 2018/ my 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. Attend ACS meetings in Boston, August 2018. Attend IUPAC and InChI and InChI Trust meetings. Meet with groups to discuss adoption and usage of InChI.
3. Invited lecture State University Stony Brook, 60<sup>th</sup> Anniversary Chemistry Department, October 2018
4. Attend the November 2018 GDCh conference and present an InChI poster.

Steve Heller

### **Reconstitution of the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature**

- 1.0 Future arrangements for joint IUPAC-IUBMB nomenclature activities were considered by the IUPAC Bureau in September 2002, and a three-person working group was appointed to open discussions with IUBMB. This group, consisting of IUPAC's Executive Director (John Jost) and Secretary General (Ted Becker) and myself, made contact with IUBMB Officers by e-mail, and discussions took place with the IUBMB Secretary General (Jacques-Henri Weil), President (Brian Clark), Treasurer (Brian Beechey), and Publications Committee Chairman (Angelo Azzi), during January-March 2003. Dick Cammack (Chairman, JCBN) was involved during final discussions over new terms of reference.
- 2.0 It became clear very soon that IUBMB wished to maintain NC-IUBMB as an entity separate from any joint body. This being so, it was agreed that JCBN needed to continue in something like its present form. However, IUPAC wished to modify funding arrangements so as to be able to assign more money directly to approved projects and less to "operational" matters (e.g. annual meetings of the full Commission). It was therefore agreed that, instead of eight Titular Members (four from each Union) and eight Associates, the Commission should consist in future of four titular Members (two from each Union) and eight Associates. One of the Titular Members (appointed by IUBMB) would be the Chairman, and another (appointed by IUPAC) would be the Secretary. The Chairman would be an ex-officio member of the IUPAC Division VIII Committee, with participation funded by IUBMB.
- 3.0 There would still be a need for an annual meeting, most conveniently held in conjunction with NC-IUBMB, for which only Titular Members would have guaranteed funding.
- 4.0 As now, NC-IUBMB would be responsible for maintaining the Enzyme List, with advice from IUPAC members of JCBN on systematic naming etc.
- 5.0 A mechanism for approval and management of projects was agreed. Under IUPAC's new project-based system, all projects are formulated as proposals for consideration by the appropriate Division Committee. Each Division has a biennial budget that can be assigned to approved projects, and some of the funding currently assigned by IUPAC to JCBN will be added to this, with the intention that the combined sum can be requisitioned for suitable projects over the whole range of chemical nomenclature, including projects arising from JCBN. JCBN projects will be funded jointly by the two Unions, and a mechanism for requesting corresponding funds from IUBMB was agreed.
- 6.0 Terms of reference for the new JCBN are attached, and will take effect from January 1st 2004.

Alan McNaught  
17 June 2003

## **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.

### **Terms of Reference**

#### *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.



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 Vohlidal	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	<i>exOfficio</i>	2016-2019	UK
Prof. Richard Hartshorn	<i>exOfficio</i>	2016-2019	New Zealand
	10 TMs, 6 AMs, 10 NRs		

11 October 2017

## Publications since the last meeting in Sao Paulo (July 2017)

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

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**, (2018), <https://doi.org/10.1515/pac-2013-0919>.

After the meeting finally printed in *Pure Appl. Chem.* **90**(9), 1429 – 1486 (2018)

J. Duffus, D. M. Templeton, M. Schwenk, *Comprehensive Glossary of Terms Used in Toxicology*, Royal Society of Chemistry, 2017 (contains a 35 pages appendix of systematic names for drugs and agrochemicals, thoroughly corrected by the President of Division VIII). See also *Chem. Int.* **40**(3), 38 – 39 (2018).

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

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

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

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

After the meeting finally printed in *J. Chem. Inf. Model.* **58**(9), 1755 – 1765 (2018)

### Translations:

K.-H. Hellwich, K.-M. Roy, Herkunftsbezogene Nomenklatur für einstrangige Homo- und Copolymere, *Angew. Chem.* **130**, 2756 – 2773 (2018) [translation from: *Pure Appl. Chem.* **88**, 1073 – 1100 (2016)]