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

Approved Minutes for Division Committee Meeting
Sao Paulo, Brazil, 8–9 July, 2017

1 Welcome, introductory remarks and housekeeping announcements

Karl-Heinz Hellwich (KHH) welcomed everybody to the meeting, extending a special welcome to those, who were attending the Division Committee (DC) meeting for the first time. He described house rules and arrangements during the meeting.

2 Attendance and apologies

Present: Karl-Heinz Hellwich (President, KHH), Risto S. Laitinen (Secretary, RSL), Osman Achmatowicz (OA), Robin Macaluso (RM), Gerry P. Moss (GPM), Michelle M. Rogers (MMR), Molly A. Strausbaugh (MAS), Andrey Yerin (AY), Ana Maria da Costa Ferreira (ACF), Amélia Pilar Rauter (APR), Fabio Aricò (FA, day 2), Jiří Vohlídal (JV, day 2)

Apologies: Michael A. Beckett (MAB), Ture Damhus (TD), Phil Hodge (PH), Alan T. Hutton (Vice President, ATH), Keith Taylor (KTT), Ebbe Norlander (EN), Gernot Eller, Martin Putala, Elisabeth Mansfield (EM)

Observers and visitors: Suthiweth T. Saengchantara (young observer, day 1, morning), Pietro Tundo, Jan Apotheker, Mustafa Sözbilir, Richard M. Hartshorn (RMH), Leah McEwen (LRM), Qi-Feng Zhou (Vice President of the Union), M. Clara Magalhães (Division V)

No replies: Ivan Dukov, Hyo Won Lee

3 Introduction of attendees

A short round of introductions was made. Prof. Ana Maria da Costa Ferreira (NR, University of Sao Paulo) and Dr. Suthiweth T. Saengchantara (young observer) attended the meeting of the Division Committee for the first time.

4 Approval of agenda

Agenda was approved (Appendix 1).

5 Approval of minutes of meeting in Cambridge, UK, 4–5 August 2016

The minutes were approved after correction of some typographical errors.

6 Matters arising

No matters were arising.

7 Interactions between Division VIII (Chemical Nomenclature and Structure Representation) and other (IUPAC) bodies in relation to documents and projects involving chemical nomenclature and structure representation.

It was decided to continue the practice started in Bangor in 2014 that there should be contact persons for interdivisional information exchange. The existing contacts were reviewed and modified, as needed. Furthermore, new contact persons were nominated for interactions between Division VIII and Division V, as well as Division VIII and Division VII. The contact persons are as follows:

Division I. The contact person is Andrey Yerin (Division I counterpart is Roberto Marquardt). He reported that there was no contact during the past year. GPM: The overlap between the Divisions is minimal and covers only the introductory comments in the Green Book.

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

Division III. The contact person is Amélia Pilar Rauter, who is also the Secretary of Division III.

Division IV. The contact person is Karl-Heinz Hellwich (the Division IV counterpart still unclear). Both KHH and PH are members of SPT providing natural overlap.

[Secretary's note: PH is not a member of Division VIII from 2018 on]

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

Division VII. Contact persons to be established

Actions: Contact relationships need to be renewed. RSL will contact the Secretaries of the above-mentioned Divisions to confirm these decisions.

ICTNS. GPM is the titular member and TD the representative of Div. VIII on ICTNS. KHH reported that all Division Presidents will meet in Sao Paulo. He said that 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 period in ICTNS is ending at the end of the year. There are several documents in process, they all need to be checked for nomenclature – also in the future. As noted last year in Cambridge (see item 7.2 in the DC minutes in Cambridge), there are problems in handling of the documents during the ICTNS phase, which has resulted in a number of errors and delays in the publication. This could be avoided, if manuscripts were circulated before submission.

CPCDS (Committee on Printed and Cheminformatics Data Standards): CPCDS is a Standing Committee of IUPAC. LRM attended the meeting of CPCDS during the GA in Busan. AY is a member of the Subcommittee on Cheminformatics Data Standards (SCDS). They are involved in the new website of IUPAC and InChI. In a recent meeting CPCDS expressed interest in closer contacts with Div. VIII. Of particular relevance is the project on InChI of mixtures (CPCDS wanted to review it). The contacts with the InChI Subcommittee also need to be intensified. In a recent meeting in conjunction of the annual meeting of CPCDS, Div. VIII was not invited or informed even though the meeting was concerned with structure representation. This work is directly related to Division VIII.

The goal of the SCDS is to work also with other bodies than IUPAC. The work is only concerned with digitalization.

The interaction of CPCDS and Division VIII should be intensified (see also item 9.13).

ISO: KHH reported that there have been no new developments since Cambridge.

CCDC. The members of the DC met with representatives of CCDC in last August in Cambridge. As a result of this meeting, CCDC has nominated Clare Tovee as an AM to the Division.

Wikipedia. KHH: In Germany there is currently a chemistry editorial board for the German pages of Wikipedia. The board has asked for help in matters concerning chemical nomenclature.

JCBN. GPM is the chairman of JCBN, and TD and APR are Associate Members, KHH ex officio member until the end of 2017 and expects to continue as AM in 2018.

Cross-over meetings on Sunday, July 9:

Cross-over meetings at 10.30 Division II-VIII and Division IV-VIII (simultaneously), and 11.30. Division VII-VIII. A change has been proposed to avoid conflicts (Division IV-VIII moved from 11.30 to 10.30). The attendees in different meetings will be decided later (Div. II RSL and RM, Div. IV KHH, Div. VII KHH).

8 Updates on Division VIII projects

8.1 IUPAC International Chemical Identifier (InChI) projects

A report by Steve Heller together with the list of current projects is presented in Appendix 2. AY reported that there will be a discussion at the ACS National Meeting in Washington, DC on August 16-18 concerning all aspects of InChI (InChI trust will meet during the last day).

Action: AY will produce a summary report of the meeting.

8.2 Preferred names in the nomenclature of organic compounds (the Blue Book)

KHH: There was a long Blue Book meeting in Cambridge last year, where several problems were recognized. GPM has produced the errata online and he is still going through the list of reported

errors and correcting these errors. During the last year, there were few comments from the task group members. The task group met in Sao Paulo (5-7 July). It was decided to put the list of corrections online provisionally. There are very many errors (1500 errors in the public list and ca. 1500 in process). There are further inconsistencies (for instance, should hydroxylamine be considered as a non-functional parent). This kind of corrections will provide separate lists in the online corrections.

The new Blue Book has reintroduced the term "thio", which was abandoned in the 1993 Guide. It was decided then that "methylsulfanyl" should be the norm, but while "methylthio" is not recommended, it should be noted that it is being used.

A number of smaller items were resolved, but there were other items, such as the inconsistent treatment of enclosing marks, for which the discussion and resolution was still postponed.

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

KHH: This project should be finished this year. Because of the inconsistencies in the Blue Book, this technical report is also dependent on the corrections therein. The completion of this technical report is anticipated to help to resolve the inconsistencies in the Blue Book.

8.4 Nomenclature of cyclic peptides (2004-024-1-800)

GPM: No progress to report.

8.5 Nomenclature of Homodetic Cyclic Peptides Produced from Ribosomal Precursors (2015-003-2-300)

GPM: The report has been published in *Biopolymers*, under the title *Pept. Sci.*, **106**(6), 917-924 (2016), but it has not gone through ICTNS, therefore it is not an IUPAC recommendation.

8.6 Nomenclature of flavonoids (2009-018-2-800)

GPM: This is a long-standing project, which should be finished during this General Assembly. KHH reported that APR should have resubmitted the document right before the meeting, but the revisions, in particular one additional example was not added in time. KHH communicated his comments (on the first *ca.* 60 pages) to APR, but did not have time to complete the commenting on the whole document (*ca.* 65 pages + appendices) before the deadline.

8.7 Revision and extension of IUPAC recommendations on carbohydrate nomenclature (2012-039-2-800)

GPM: A large document is being produced. There was a two-and-a-half-days meeting in connection with the JCBN meeting. Substantial progress has been made in recent years. The symbolic representation of carbohyrates has been resolved. Two schemes have been proposed. The budget has been consumed. A proposal for the extension of the project has been submitted.

8.8 Glossary of small molecules of biological interest (2009-022-2-800)

GPM: 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 only a simple document for some important small molecules of biological interest. Not for a full large database. The chairman, Marcus Ennis, who had taken this project over from Dick Cammack, has resigned from all JCBN and related tasks earlier this year. Gareth Owen was nominated to replace him.

8.9 Nomenclature of phosphorus-containing compounds of biochemical importance (2006-019-1-800)

KHH: For this project a new chair needs to be found. KHH also remarked that we were reminded by RMH that the projects that are incomplete but which are not being worked on should be declared closed. GPM: There are actually two projects, which never had a budget, but which now need to be applied for as a new project, if the work is to continue (see Item 8.5 in the Cambridge minutes of 2016).

8.10 Preferred names for inorganic compounds (2006-038-1-800)

This project is divided into two aspects. Selection and priorities of central atoms and the development of the kappa convention. RMH became Secretary General of IUPAC and TD took up the project. A general problem is the use of locants in connection with the kappa convention. It became obvious that the ligand names need to be modified in certain situations. Therefore naming the ligand may become more complicated, while assembling and placing kappa-terms becomes simpler.

TD started to write a new document and recognized similarities in the treatment of isotopically modified species in the Blue Book. The consequences still need to be worked out (see Item 8.24).

8.11 Brief guides to the nomenclature of organic and inorganic chemistry ('Essentials' of organic and inorganic nomenclature) (2010-055-1-800)

KHH: The Brief guide to the nomenclature of inorganic chemistry has been published in 2015 and reprints and a poster have been presented at several chemical conferences. The poster will also be presented at the IUPAC World Chemistry Congress 2017 in Sao Paulo and 300 copies of the Brief Guide will be available for distribution.

The organic Brief Guide causes more problems. Formulae are larger and therefore there is less space for text. The meeting in Cambridge saw several improvements. The text needed to be reduced. KHH inserted all changes and this part of the work is complete. There is now some further space available for additions, if needed.

8.12 Nomenclature for polyhedral boranes and related compounds (2012-045-1-800)

A document was in Divisional review and MAB has taken the comments into account. The positions of locants, when the species is a ligand again became problematic (see Item 8.24).

8.13 Nomenclature for metallacycles containing transition metals (2013-030-1-800)

ATH: The metallacycle task group has produced a substantial draft document, but there has been no progress since the Cambridge meeting, because the final formulation is dependent on the developments around the kappa, Inorganic PINs, borane and Blue Book revision projects (see Item 8.24).

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

KHH: There is no new information. The document should be close to publication. It has to be clarified with Division II.

8.15 Terminology and nomenclature of inorganic and coordination polymers (2011-035-1-800); for short TINCOPS

The TINCOPS task group had a very fruitful meeting in Canterbury in August 2016, hosted by the chair, Richard Jones. A plan was made for how to progress a new document that would have freshly drawn structural diagrams and nomenclature and terminology updated according to the Red Book 2005 as applicable and the latest developments of the kappa notation for specifying ligating atoms in ligands.

In the first weeks after the meeting there was quite some E-mail correspondence dealing with various poblems that still needed clarification, and some of this correspondence was shared with members of the staff at the Cambridge Crystallographic Data Centre, with whom members of Division VIII had met in Cambridge in connection with the Division VIII annual meeting (just before the Canterbury meeting).

Problems that the group has discussed and which still need more work include the precise use of italicisation, hyphens and enclosing marks in connection with prefixes like catena, poly, phyllo, catena-poly, star-poly, *etc.*; some terminology matters that have to take into consideration also what has been done in other documents in the polymer area; and some (seemingly) conflicting prescriptions regarding element sequences (such as needed when ordering central atoms for additive naming and for ordering heteroatoms in organic ligands) when referring to the Red and Blue books. Regarding the kappa convention, the TINCOPS group awaits the developments in the Division VIII task group on that topic.

The nature of the source document from 1985 made it necessary more or less to start all over for preparing a new document, and there have been technical issues regarding the exchange of particular formats of structural drawings between group members and implementation of a reference system, but these seem to have been more or less resolved.

8.16 Polymer projects (with Division IV)

8.16.1 Source-based nomenclature of single-strand organic polymers (2003-042-1-800)

KHH: This is a long-standing project. The document was published in November 2016. A few minor errors were introduced during the production. It is the first polymer nomenclature document that is consistent with organic-chemical nomenclature. The appendix contains a table with a

correlation of structure-based names and source-based names. The concept of retained polymer names has been introduced (equivalent to trivial names).

8.16.2 Terminology and structure-based nomenclature of dendritic and hyperbranched polymers (2001-081-1-800)

KHH: The document has been through public review and has just finished the second review by ICTNS. There were a few minor points raised by one reviewer.

8.16.3 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)

KHH: The document was under review at the end of last year and went back to ICTNS and to a second review. Shortly thereafter the document was accepted under the title "Preferred names of constitutional units for use in structure-based names of polymers" and the first proofs have been seen. Several errors were introduced by the typsetter and the tables were misplaced. The second version of the proofs should be coming.

8.16.4 Revision of IUPAC Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology (2008-020-1-400) (Web-based IUPAC recommendations on polymer nomenclature)

KHH: There is a document with completely revised text and formulae. The draft should be finalized in Sao Paulo. The structure corrections are still incomplete and there is no uniformity. The question is, how to finish the document without the chairman attending the meeting (PH). The document now has the thitle "IUPAC Recommendations on Polymer Nomenclature, A concise guide to polymer nomenclature for authors of papers and reports in polymer science and technology".

8.16.5 Definitions and notations relating to stereochemical aspects in polymer science (2009-047-1-400)

KHH: Since the Istanbul meeting in 2016, there have been at least 6 versions (with some more versions with minor annotations), which need to be reviewed by the task group. To finish the project, these different versions need to be assembled into one final document which is a supplement to the existing 1981 document revising it.

8.16.6 Structure-based nomenclature for regular star and brush polymers (2013-031-3-800)

KHH: The document was in review at the beginning of 2017. There were several comments from Division VIII, none from SPT. A revised version was circulated a few days ago. It will be discussed during the SPT meeting.

8.16.7 Nomenclature for polymeric carriers bearing chemical entities with specific activities and names (2014-034-2-400)

GPM: There is a new document, which came around recently. AY: It is better but still needs modification.

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

KHH: There is a published document, but it needs corrections. Nothing new since last year.

8.17 End-of-line hyphenation of systematic chemical names (2014-003-2-800)

KHH reported that before the Cambridge meeting he had revised certain sections and communicated with the chairman of the task group. However, because of misunderstandings, important information has been lost in the revised document circulated before the Sao Paulo meeting. The new version is not instructive and still needs further work.

8.18 Nomenclature of carbon nanotubes and related substances (2013-056-1-800)

AY: A core document exists. There will be no meeting in Sao Paulo. The document will be worked on, and the task group will meet in the near future. The nomenclature needs to be harmonized. It has been decided to classify carbon nanotubes according to their sizes and number of walls. There is a need for a system to describe configuration and isomerism, functionalization, etc.

8.19 Solid State terminology (2015-053-1-200)

RM: The project is now running for one and a half year and it is progressing as planned. The first face-to-face meeting took place in Sao Paulo. The document was presented and discussed. The naming of solids is complicated. The project started by considering the crystalline solids and looking at different bonding types. Everybody in the task group has been given a task. The next meeting is in November through skype. There is an educational component in the project. However, since the International Year of Crystallography, IUCr has created plenty of teaching material and the task group will not repeat this work. In terms of creating websites, cooperation with other bodies is more effective than doing it alone. Collaboration with material chemists might be a possibility. Focus is also on the college (undergraduate) level.

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

LRM: This project has been closed and will be replaced by a new project.

8.21 Nomenclature of Transition States and their Analogs for Phosphoryl Transfer Reactions (2013-039-2-300)

GPM: The document has been published in PAC in 2017 [*Pure Appl. Chem*., 2017, **89**(5), 653-675].
KHH: The authors were alerted for deviations from IUPAC Red Book recommendations. They added a footnote that the IUPAC recommendation is different. It was stated in 1976 that phosphoryl should be used as in RB, but this document is in deviation from this usage. GPM: enzymologial nomenclature is different from chemical nomenclature.

8.22 Graphical representation standards for chemical reaction diagrams (2003-045-3-800/2012-033-1-800)

KHH: There is no prgress during the last year. A project proposal should be imminent.

8.23 Protecting groups abbreviations project (2011-044-1-300)

KHH: There is nothing new to report.

8.24 Alignment project

KHH: The problem with kappa and locants and its consequences needs to be resolved. Since ATH, TD, MAB are not present in the Division Committee meeting in Sao Paulo, and it was not possible to have a meeting before Sao Paulo, it has been decided to have a longer meeting in November leading to the application for a new project. The members in this task group should be people involved in the kappa, borane, metallacycle, and TINCOPS projects, among others. The ideal is a three-day meeting to review all areas, where these problems appear. This includes, in addition to ligands, also isotopically modified molecules. The objective is to agree with general features and the meeting is long enough to solve all problems. Possibly then borane and metallacycle documents could be speedily completed.

9 Future projects/activities

9.1 International Standards Organization (ISO) liaison. Nanoparticles projects (see also 8.18 above).

KHH: There are no new developments. There have been some contacts with Ed Constable, but not with representatives of ISO.

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

RSL: This project should be initiated. It is important to identify sections needing revision. A project proposal should be made in the near future.

9.3 Graphical representation of polymers.

KHH: There is nothing new to report. It is a long-lasting idea. The involvement of Division IV is essential (JV will contact Division IV). During the cross-over meeting with Div. IV, it was agreed that this project should be started during the next year.

9.4 Rotaxane stereochemistry.

AY: There is nothing to report. People working in this field are not interested.

9.5 Delocalised systems.

AY: There is nothing new to report.

9.6 Crown nomenclature, calixarenes.

There is nothing new to report. Currently there is no need for new nomenclature. Possibly only a Technical Report should be created.

9.7 Central webpage for all IUPAC recommendations/publications.

KHH: This question is becoming more urgent. The structuring and searching of material needs to be developed (see Item 9.7 in the Cambridge minutes 2016).

9.8 Document on italic and roman fonts.

KHH: There is nothing new to report.

9.9 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.

The project is on hold. Background is needed. Kappa- and other issues need to be resolved.

9.10 Variable substitution.

There is nothing new. The same problems as in item 9.9.

9.11 IUPAC terminology for recommended, acceptable, not acceptable names etc.

There is nothing new to report. This item must involve also other IUPAC bodies.

9.12 Overall numbering of atoms of a compound.

There is nothing to report. AY: There could be interest in this topic in CPCDS, CCDC and in the Analytical Chemistry Division.

9.13 Colour Book for Cheminformatics Standards.

Report and presentation by LRM (see Appendix 3). KHH was the only one, who sent the evaluation for the project proposal. One of the problems had been that it was not clear, what the project was about. Now the presentation makes the project proposal clearer and it was considered that this is a worthwhile project. It has to be stated clearly that it is a scoping project with everything else as background information.

9.14 Other projects.

9.14.1 Webpage format of Brief Guides

RM proposed that Brief Guides should be converted also to phone-format. KHH commented on the problem with cross-references. RSL noted that since the printed document and the webpage-document need not be mutually exclusive, they can present the information in different ways. Pros and cons were discussed.

9.14.2 Project on liquid crystals

KHH: There was a project proposed last year. In the reviews it was pointed out that the project did not bring anything new to nomenclature and therefore cannot be a Division VIII project. Another

problem was that the project was not international enough. It should be a project for Divisions II or III, but they are apparently not interested.

9.14.3 Unicode for chemistry

KHH reported that he was approached and asked by a publisher that there is no Unicode for chemistry and whether this would not be an appropriate project for IUPAC. While this is a project for CPCDS, it also has interdivisional character. AY: For names the most critical points in some applications are the special fonts, super- and subscripts, etc. Tags must be supported. KHH: The IUPAC project is the definition of symbols to be included in the chemistry unicode. Their programming is a different matter.

Action: CPCDS, PAC, and ICTNS should be approached

9.14.4 Project with CCE

Jan Apotheker and Mustafa Sözbilir from CCE visited the meeting. CCE is working in the chemistry education program in countries where it is less developed. There is need for cooperation. He questioned, whether any of the CCE activities are interesting for Div. VIII. It was concluded that nomenclature needs to be explained both to teachers and students and there could be short projects on lower level nomenclature. CCE can help in creating suitable material.

10 Visit by the Interdivisional Committee on Green Chemistry for Sustainable Development

Pietro Tundo from the Interdivisional Committee on Green Chemistry for Sustainable Development visited the meeting. He described a problem the Green Chemistry Committee is facing in chemistry publications. Most papers claiming to be Green Chemistry are not always green or green only to a small extent. IUPAC should establish metrics to decide, whether the project or a publication is green or not. There is a draft proposal, which Division III agrees to be a part of. The solution to this dilemma is not easy. The Committee discussed the possible involvement of Division VIII but made no decisions.

11 Visits by The Secretary General and The Vice-president of IUPAC

11.1 Visit by the Secretary General

KHH welcomed the IUPAC Secretary General, Richard M. Hartshorn, who made the introductory comments:

(1) He emphasised the importance of succession planning and the need to look for new members on longer terms (escpecially officers). New people need to come in all the time. Young Observers are important and need to be retained.

(2) RMH drew the attention to the new interdivisional organization: Green Chemistry, which is an important field. It is also important to evaluate, whether old Divisions are still needed. The Divisions should look at the IUPAC strategic plan. Division rules need to be developed, which describe the way Divisions work. The Council should approve these rules in 2019. Division V has

clear descriptions of the duties of TM, AM, NR, etc. For instance, it should be noted in the rules that a representative from CAS should be a member. There could be a need to define the number of common members in different Divisions, as appropriate.

KHH observed that the question of turnover is important and critical in nomenclature. One cannot have the necessary experience during the project duration of 2 – 4 years. RMH: (1) Exceptions are always possible. (2) Task group leaders are always welcome in DC meetings. (3) The Division President is enpowered to give extra funding to extend the time of a task group member for DC meeting. (4) There can be an application to change the statutes, if needed.

11.2 Visit by the Vice-President

The Vice President of IUPAC, Professor Qi-Feng Zhou paid a short visit to the meeting of Division VIII. KHH welcomed him and described briefly the activities within the Division. After a brief introduction and discussion, Prof. Zhou observed the ongoing discussion in the meeting.

12 Reports from cross-over meetings

12.1 Divisions II and VIII

Present:

Division II: Jan Reedijk, Lars Öhrström, Markku Leskelä, Tipping Ding, Dan Rabinovich, Thomas Walczyk

Division VIII: Osman Achmatowicz, Risto Laitinen, Robin Macaluso, Michelle Rogers, Molly Strausbaugh

12.1.1 Introductions and welcome (Reedijk)

Jan Reedijk, president of Division II, was appointed as a chairman of the meeting. He welcomed the participants and a round of introductions was made.

12.1.2 Agenda was distributed earlier by Reedijk and was approved.

12.1.3 Risto Laitinen and Markku Leskelä were appointed to take the minutes.

12.1.4 Division VIII did not bring any special items for discussion.

12.1.5 Items brought in from Division II actions were discussed.

(a) The short 4-page “Brief Guide to the Nomenclature of Inorganic Chemistry” may need some clarifications. The document is short and has turned out to be a bit difficult for teachers. Specially, the snake table needs more detailed explanations. It was also discussed that this document and its future counterpart “Brief Guide to the Nomenclature of Organic Chemistry” should be formatted to suit better for use with smartphones and tablets. This would apply also to the IUPAC webpage, since the young generation wants to have everything easily available in their phones.

(b) The status of the joint projects (coordination polymers, kappa document, inorganic PINs, polyhedral boranes, metallacycles, solid state chemistry terminology) was reviewed. The consistent application of the kappa-convention has turned out to be problematic and most of the above-mentioned projects are waiting for its satisfactory solution. The task group of the project will meet in November and hopefully find a solution to the problem.

(c) Revision of the Red Book is needed and that is on the to-do list of Division VIII.

(d) Periodic Table issues were discussed. There are a few projects going on about the PT of which the project of Scerri can be mentioned. That project is dealing with the position of lutetium and lawrencium in the Periodic Table. In the centenary activities of IUPAC the Periodic Table may play a role because the year 2019 has been proposed as International Year of the Periodic Table.

12.1.6 Mary Garson visited the meeting and told about the IUPAC centenary committee. She will coordinate the actions for that year and all suggestions for activities should go via her.

12.1.7 The chairman acknowledged the participants for the discussions and ended the meeting.

12.2 Divisions III and VIII

A very brief event in which RSL attended the regular meeting of Division III and described the main projects active in Division VIII. The Blue Book revision naturally aroused the main interest, and a brief discussion took place. No particular items were brought into discussion.

12.3 Divisions IV and VIII

A round table discussion was conducted about suitable projects. Many different things were raised, most of which were beyond current nomenclature. The problem is the number of building blocks. Possible projects of mutual interest: Graphical representations of polymer structures. Electronic representations of polymer structures, but this is the project of CPCDS. Two years ago it was agreed to compile lists of memberships in the two Divisions and their expertise. This still needs to be done.

12.4 Divisions VII and VIII

The members of Division VII had a few specific questions on drawing formulae and on naming, which could be answered (not necessarily to their satisfaction). It was suggested to avoid implied configuration. There are severe problems with complex structures of drugs, etc. (D. Templeton's book is helpful here). There are several inconsistencies and ambiguities with complex structures. The list in the book has ca. 100 compounds with verified structures and correct systematic names. The request should come earlier than at the proofs stage.

13 Membership matters

13.1 Status of Division VIII Committee membership

KHH: As this is the General Assembly year, the Titular Member elections, Associate Member selections, and National Representative appointments need to be made. There was a number of

nominations, but in many cases, the cv did not indicate background in nomenclature or structure representations. However, Division VIII has a full roster. (Appendix 4)

13.2 Division VIII representatives in other IUPAC bodies

CCE:	RM
PAC Editorial Advisory Board:	KHH
ICTNS:	TD
COCI:	MMR is the contact person
JCBN:	KHH will put forward a nomination of Gareth Owen as a new IUPAC-funded TM of JCBN (as replacement for Marcus Ennis who resigned earlier this year). APR (AM), TD (AM), KHH (ex officio)
CPCDS:	KTT, AY are members of the Subcommittee (SCDS), LRM is the chairman.
Interdivisional Committee on Green Chemistry for Sustainable Development:	FA is member and the natural contact person.

13.3 Division VIII Advisory Subcommittee

The membership was reviewed, as agreed in 2016. After that nothing has happened.

13.4 Nominating committee

The chair and the members of the Nominating Committee should be nominated well in advance (2-3 from DC and 2-3 outside members)

14 Division Rules

Only Division VII had Division Rules (from 2009). They were reviewed. The Division President has the right to invite people for special reasons to meetings, provided there is sufficient funding. There was a discussion about the nomination, appointment, and removal of members. Expertise, balance, etc. is needed. The NAOs need to be made aware of this. It was proposed to formulate specific duties for TMs, AMs, and NRs.

15 Status on Division VIII web board with discussion forums

There is nothing new to report.

16 Publicity

16.1 Division VIII (and related) publications since the 2016 Division Committee meeting

See Appendix 5.

16.2 Translations

Blue Book: Japanese

Red Book: The Portuguese translation is close to completion; it is currently in the proof stage.
Inorganic Brief Guide: Portuguese (intended), Basque, Galician, Dutch, Danish, Spanish.

16.3 IUPAC-IUBMB nomenclature website

GPM: The main changes on the site concern with the Blue Book revision. The Blue Book has now also been published in Japanese. Details of the Portuguese version of the 2005 Red Book have been provided on the webpage.

16.4 IUPAC website

The website has been improved, but needs development in mobile format. The login function is now working. There will be a possibility to add content and every person can change their profiles. MMR voluteered to act as webpage contact person.

17 Reports from other IUPAC bodies

17.1 ICTNS

See Item 7.

17.2 JCBN

JCBN met on May 11 in Killarney, Ireland. See Items 7 and 13.2, and the project reports 8.7, 8.8, 8.9.

17.3 CCE

See Item 9.14.4.

17.4 CPCDS

See Items 7 and 9.13.

18 Any other business

There was no other business.

19 Dates and venue for next meeting

The meeting times and venue were discussed. Possible places could be Basel, Switzerland and Cambridge, UK. The meeting should take place in August taking possible conflicts with conferences into account. Meeting in conjunction with the ACS National Meeting was also considered.

20 Adjournment

KHH thanked everybody for attendance and contributions and the hard work during the meeting. The meeting was adjourned at 16.27.

Appendix 1

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

Draft agenda for Division Committee Meeting
Sao Paulo, Brazil, 8–9 July, 2017

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 Cambridge, UK, 4–5 August 2016

6 Matters arising

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

8 Updates on Division VIII projects

8.1 IUPAC International Chemical Identifier (InChI) projects

8.2 Preferred names in the nomenclature of organic compounds (the Blue Book)

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

8.4 Nomenclature of cyclic peptides (2004-024-1-800)

8.5 Nomenclature of Homodetic Cyclic Peptides Produced from Ribosomal Precursors (2015-003-2-300)

8.6 Nomenclature of flavonoids (2009-018-2-800)

8.7 Revision and extension of IUPAC recommendations on carbohydrate nomenclature (2012-039-2-800)

8.8 Glossary of small molecules of biological interest (2009-022-2-800)

8.9 Nomenclature of phosphorus-containing compounds of biochemical importance (2006-019-1-800)

8.10 Preferred names for inorganic compounds (2006-038-1-800)

8.11 Brief guides to the nomenclature of organic and inorganic chemistry ('Essentials' of organic and inorganic nomenclature) (2010-055-1-800)

8.12 Nomenclature for polyhedral boranes and related compounds (2012-045-1-800)

8.13 Nomenclature for metallacycles containing transition metals (2013-030-1-800)

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

8.15 Terminology and nomenclature of inorganic and coordination polymers (2011-035-1-800); for short TINCOPS

8.16 Polymer projects (with Division IV)

8.16.1 Source-based nomenclature of single-strand organic polymers (2003-042-1-800)

8.16.2 Terminology and structure-based nomenclature of dendritic and hyperbranched polymers (2001-081-1-800)

8.16.3 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)

8.16.4 Revision of IUPAC Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology (2008-020-1-400)

8.16.5 Definitions and notations relating to stereochemical aspects in polymer science (2009-047-1-400) (Web-based IUPAC recommendations on polymer nomenclature)

8.16.6 Structure-based nomenclature for regular star and brush polymers (2013-031-3-800)

8.16.7 Nomenclature for polymeric carriers bearing chemical entities with specific activities and names (2014-034-2-400)

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

8.17 End-of-line hyphenation of systematic chemical names (2014-003-2-800)

8.18 Nomenclature of carbon nanotubes and related substances (2013-056-1-800)

8.19 Solid State terminology (2015-053-1-200)

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

8.21 Nomenclature of Transition States and their Analogs for Phosphoryl Transfer Reactions (2013-039-2-300)

8.22 Graphical representation standards for chemical reaction diagrams (2003-045-3-800/2012-033-1-800)

8.23 Protecting groups abbreviations project (2011-044-1-300)

8.24 Alignment project

9 Future projects/activities

9.1 International Standards Organization (ISO) liaison. Nanoparticles projects (see also 8.18 above).

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

9.3 Graphical representation of polymers.

9.4 Rotaxane stereochemistry.

9.5 Delocalised systems.

9.6 Crown nomenclature, calixarenes.

9.7 Central webpage for all IUPAC recommendations/publications.

9.8 Document on italic and roman fonts.

9.9 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.

9.10 Variable substitution.

9.11 IUPAC terminology for recommended, acceptable, not acceptable names etc.

9.12 Overall numbering of atoms of a compound.

9.13 Colour Book for Cheminformatics Standards.

9.14 Other projects.

10 Visit by IUPAC Secretary General

11 Membership matters

11.1 Status of Division VIII Committee membership

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

11.3 Division VIII Advisory Subcommittee

12 Division Rules

13 Status on Division VIII web board with discussion forums

14 Publicity

14.1 Division VIII (and related) publications since the 2016 Division Committee meeting

14.2 IUPAC-IUBMB nomenclature website

14.3 IUPAC website

15 Reports from other IUPAC bodies

15.1 ICTNS
15.2 JCBN
15.3 CCE

16 Any other business

17 Dates and venue for next meeting

17 Adjournment

Name	Status	Term	NAO
Dr. Karl-Heinz Hellwich	President	2014-2017	Germany
Prof. Alan T. Hutton	Vice President	2016-2017	South Africa
Prof. Risto S. Laitinen	Secretary	2016-2019	Finland
Prof. Osman Achmatowicz	TM	2016-2017	Poland
Dr. Ture Damhus	TM	2016-2017	Denmark
Prof. Philip Hodge	TM	2016-2017	United Kingdom
Prof. Robin Macaluso	TM	2016-2017	USA
Prof. József Nagy	TM	2016-2017	Hungary
Dr. Michelle Monnens Rogers	TM	2016-2017	USA
Prof. Jiří Vohlídal	TM	2016-2017	Czech Republic
Prof. Michael A. Beckett	AM	2016-2017	United Kingdom
Prof. Ivan L. Dukov	AM	2016-2017	Bulgaria
Dr. Gernot A. Eller	AM	2016-2017	Austria
Dr. Elisabeth Mansfield	AM	2016-2017	USA
Dr. Keith T. Taylor	AM	2016-2017	USA
Molly A. Strausbaugh	AM	2016-2017	USA
Dr. Fabio Aricò	NR	2016-2017	Italy
Prof. Ana Maria da Costa Ferreira	NR	2016-2017	Brazil
Prof. Alain Fradet	NR	2016-2017	France
Prof. Hyo Won Lee	NR	2016-2017	Korea
Prof. Todd L. Lowary	NR	2016-2017	Canada
Prof. Ebbe Nordlander	NR	2016-2017	Sweden
Prof. Martin Putala	NR	2016-2017	Slovakia
Prof. Amélia Pilar Rauter	NR	2016-2017	Portugal
Jan Pieter van Lune	NR	2016-2017	Netherlands
Dr. Andrey Yerin	NR	2016-2017	Russia
Prof. Richard M. Hartshorn	*Ex Officio*	2016-2017	New Zealand
Dr. Gerard P. Moss	*Ex Officio*	2016-2017	United Kingdom
	10 TMs, 6 AMs, 10 NRs		

Appendix 2

InChI Trust Project Director's Report

June 2017

Summary:

Since the August 2016 report there continues to be good progress with InChI and the InChI Trust in a number of areas. The final version 1.05 of the InChI algorithm was released in January. The first version of RInChI was released. The March EBI workshop on InChI was well attended and quite successful. The August NIH InChI meeting is moving forward with some three dozen registrations already submitted. More organizations, databases, and publications continue to use the InChI algorithm. Finally, Chemical Abstracts has joined the Trust.

Items covered in this report:

Membership/Support
InChI RFP/Contracts
InChI development work
IUPAC InChI subcommittee and working parties/groups
Meetings attended & Talks/ Posters given
Manuscripts
InChI Trust Web Site
InChI Usage
Technical Issues
Plans for 2016/2017

Membership/Support:

Summary

Chemical Abstracts Service has joined the Trust for 2017. IBM and PE have not paid their dues and have been removed. Discussions with EPA to join are proceeding. PLOS has expressed interest in joining but feels their amount of chemistry publications does not yet justify membership. CDISC and GBSI have not yet responded to the follow up on their joining. The same is true for EPA, Prous Research, and others.

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 June 1, 2017

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

Supporters: 47

InChI RFP/Contracts

As has been the case for a long time, the contract for Markush structures remains on hold waiting for funding

The contract for taking forward the RInChI work that Jonathan Goodman and Chad Allen did at Cambridge University with Dr. Gerd Blanke (Germany) is progressing well.

Testing of the code has now been completed by the RInChI working group and the first version released to the public,

InChI development work

Igor Pletnev continues to do a superb and a very responsive job as the InChI programmer. The work to program and respond to the many odds & ends bugs for version 1.05 took much more time than initially expected, but clearly the resulting product, while not perfect, if much better having had all the feedback and help from the community. The good news with this extensive and time-consuming effort to get v 1.05 as correct as possible is that there was considerable feedback from the community resulting in a well-tested release. And the bad news is that all this testing resulted in many things that needed to be fixed and hence the delay in the release.

IUPAC InChI subcommittee & working groups

InChI work Groups

Chemical mixture composition

Leah McEwen at Cornell University has initiated a working group for chemical mixture composition. As noted previously, recent highly damaging events in chemical laboratories and classrooms have led to increasing focus on chemical information management in laboratory organizations. The diverse teaching and research environment in the academic sector particularly is raising awareness of the complexity of chemical safety information resources and formats available. A key concern in this regard is that documentation of chemicals with current identifiers is a persistent challenge for tracking and managing chemicals across the chemical enterprise, from process planning to manufacture to waste disposal and emergency response.

The objective of this project is to establish requirements and guidelines for the generation of a unique identifier for all forms of a chemical (liquid, gas, solid, powder, etc.). Currently, many chemical identifiers exist, but very few reflect these bulk properties of substances, which may commonly exist in many forms and mixtures. Furthermore, most existing identifiers present cross-referencing challenges between systems designed around different initial applications and editorial principles.

The intended outcome of this project is global adoption of the InChI notation in chemical inventories and information systems across commercial, industrial, government, academic and educational sectors to facilitate accurate documentation, handling and exchange of chemical information in support of safer management and use of chemicals.

This project is complementary to another user-focused project that is developing a QR code version of the InChI to facilitate labeling and other communication of chemical safety information. That project will be consulting with global stakeholders to determine deployment and use approaches. This project will focus the specificity and usefulness of the information being encoded in the InChI.

This working group is probably unique for the InChI project in that it is of clear scientific value, but even of more importance and value to all the chemistry labs around the world. Safety is something that makes the front page of newspapers and TV news programs.

This project, entitled "InChI Extension for Mixture Composition" was funded by IUPAC in June 2016.

Positional Isomers

Considerable technical interest in positional isomers has developed in the past but no one was willing to take the lead for this area. Chris Steinbeck at EBI who had hoped to lead this effort was promoted and does not have sufficient time to chair the working group. However, Chris has just left the EBI to go to the University of Jena and has now agreed to lead the effort.

The current members of this working group are:

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

Resolver – No further progress report has been submitted since my last report. However, I do expect an update prior to the March Trust Board meeting.

Polymers – With release of version 1.05 a limited area of polymer chemistry can now be handled by the InChI algorithm.

Reactions –Under the programming direction of Gerd Blanke this project has moved ahead very nicely. The RInChI 1.0 release has been tested against the US patent database 2008-2011 with 420.000 reactions (provided by Nextmove) and they have not found anything that should stop the release. The worst reaction they found had 95 educts and 22 products but the RInChI was calculated without any issues. Version 1.0 has now been released.

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

Chairman: Gunther Grethe

Members:
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 occur is there is sufficient interest and need and funding.

Electronic States –. There still are no further developments here.

InChI for Materials – There is still no news from the NIST staff about this. This topic will be dropped in future reports.

Organometallics- Colin Batchelor and his working group expect a final report in 2017. They are having discussions with the Inorganic working group as there is considerable overlap.

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. –

Little has happened since the October 2014 working group meeting at NIH as Keith Taylor was waiting for the extensions of InChI past 1024 atoms. Igor has now accomplished this and Keith has tested it to his satisfaction. With this now accomplished progress will follow starting with the EBI InChI workshop in March 2017.

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

Chairman: Taylor, Keith

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

Tautomers. – Under the leadership of Marc Nicklaus, NIH/NCI, InChI project #2012-023-2-800, "Redesign of Handling of Tautomerism for InChI V2" is approved for funding by IUPAC. Marc plans to hold a working group meeting on this at the August 2017 InChI meeting at NIH.

2012-023-2-800: Redesign of Handling of Tautomerism for InChI V2
http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2012-023-2-800

Chairman: Marc Nicklaus

Members:
Bolton, Evan
Ihlenfeldt, Wolf-Dietrich
Peryea, Tyler
Pletnev, Igor
Rey, Hinnerk
Sitzmann, Markus
Tchekhovskoi, Dmitrii

Interlocking structures (rotaxanes) - There has yet to be any effort to look into how to handle these structures. This topic area will dropped in future reports until there is movement.

Extended Stereochemistry - Evan Bolton 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."

July 2016 – December 2016 activities

Meetings Attended; Talks/Posters Presented

A number of conference call meetings with David Evans, 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 fall ACS meeting in Philadelphia and had a number of productive conversations and meetings.

I chaired another InChI session at the May 2017 BioIT meeting.

Manuscripts

No new manuscripts were published in the second half in 2016 or beginning of 2017.

InChI Trust web site

The Trust web site has left the IUPAC server and is now up on the InChI Trust cloud server. Aletia Rey who was hired to maintain and add content to the web site is doing an excellent job.

InChI Usage

For lack of a better a better term, I use InChI Usage to refer to publications and blogs about InChI. Alan and I have been passing these on to Aletia and she has added these to the web site. There have been quite a number of publications using InChI. The numbers continue to grow. Searches on Google (and other search engines) continue to have more hits for InChI strings and InChIKey strings.

InChI Trust Videos - Access numbers:

InChI & the Islands – 960 (1/17); 883 (7/16); 804 (1/16); 728 (7/15); 629 views (12/14); 526 views (7/14)

The Googlable InChIKey – 1,379 (1/17); 1,203 (7/16); 1,037 (1/16) ; 915 views (7/15); 751 views (12/14); 597 views (7/14)

The Birth of the InChI - 1,365 (1/17); 1,233 (7/16); 1,084 (1/16); 984 views (7/15); 835 views (12/14); 687 views (7/14)

What on earth is InChI? - 4,188 (1/17); 3,762 (7/16) ; 3,331 (1/16); 2,956 (7/15); 2486 views (12/14); 1977 views (7/14)

IUPAC InChI (Google lecture)– 950 (1/17); 946 (7/16); 931 (1/16); 922 views (7/15)
https://www.youtube.com/watch?v=mH9fuspg_h0

Representing Chemical Structures on computer – 675 (7/16); 546 (1/16); 390 views (7/15)
https://www.youtube.com/watch?v=uzXkJ9BsyHQ
(InChI part starts at about 14 ½ minutes into the video

Scott Wiedemann
Cheminformatics, Encodings SMILES & InChI – 879 (1/17); 647 (7/16); 468 (1/16); 354 views (7/15)
https://www.youtube.com/watch?v=V9HHnRAS5BA

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 of version 1.05 prior to the 1.05 release.

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.

Plans and Activities for 2017

For 2017 my overall plans and goals are as follows:

1. Work to expand the current membership with two basic classes of members – Full and Associate, and add to the number of Supporters. Work to sign up more organizations for the Certification Suite.
2. Continue to attend meetings and give talks on InChI where useful and appropriate.
3. Attended the ACS meeting in San Francisco. Met with groups to discuss adoption and usage of InChI.
4. Attended the May 22-24, 2017 BioIT meeting and chair the InChI session at BioIT.
5. Attended the March 20-21 2017 EBI InChI industry workshop and give a lecture.
6. Attended the March 23, 2017 InChI Trust Board meeting.
7. Deliver an InChI manuscript for an upcoming issue of CI.
8. Prepare an invited talk for the ACS Washington DC meeting in August
9. Prepared a talk and poster for Ray Boucher to deliver at the IUPAC General Assembly in Sao Paulo.

Steve Heller

Appendix 3.

Cheminformatics Color Book Discussion in São Paulo

July 10, 2017

The Subcommittee on Cheminformatics Data Standards (SCDS), a subcommittee of the Committee on Publications and Cheminformatics Data Standards, will be meeting on Monday afternoon, 2-5 pm, in the Van Gogh Room at the IUPAC General Assembly. From 3-5 pm, the Subcommittee will present its ideas regarding a new Color Book on Cheminformatics and receive feedback from the community. The meeting is open to all, but we especially want to hear the perspectives of the Divisions and Committees. Publication and sharing of research data has become an important area of responsibility for researchers, as a mechanism for greater transparency in scientific research and in response to funding agency mandates. Currently there are very few digital standards for exchange of chemical data and no recognized authority for applying consistent representation of chemical data in digital formats. A Color Book for Cheminformatics could provide a guide for researchers who are required by funding agency mandates to publish and share their research data, for vendors to create software to enable better workflows for publishing data, and journal publishers and data repositories that enable storage and retrieval of chemistry data. Existing IUPAC standards, such as JCAMP-DX, ThermoML, and InChI will be an important part of the discussion.

The agenda for the Cheminformatics Color Book is:

1. Description of the project – draft of rationale and scope
• Review from previous expert workshops – needs, stakeholders

2. Proposed Timeline:
• July – December, 2017, through community workshops:
    o Define rational and scope more completely, as a new type of resource in chemistry
    o Review of current chemistry digital data standards
    o Identification of gaps and needs
    o Tentative table of contents
    o Vision for this Color Book as on online-first, digital publication
    o Line up global representation on a project committee
• December, 2017:
    o Decision whether to recommend a Color Book for Cheminformatics
• January, 2018 – July, 2019
    o Define Color Book

- o Assign teams to each Color Book Section
- o Create team to design the online, digital edition
- o Create team to create the print companion to the online edition

From 2-3pm, the formal SCDS meeting on Monday, July 10, is also open and all are welcome. We especially encourage you to join us from 3-5 pm to help us define the Color Book on Cheminformatics. Note: If you won't be attending the General Assembly, but would still like to join us, we plan to provide virtual access.

Please let us know if you have any question or suggestions. Thanks for your consideration.

Co-Chairs:
Leah McEwen (lrm1@cornell.edu), Dave Martinsen (martinsen.david@gmail.com)

Appendix 4

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INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Membership - Division (VIII)

Chemical Nomenclature and Structure Representation

2018 - 2019

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

11 October 2017

Appendix 5

Publications since the last meeting in Cambridge (August 2016)

Comprehensive Definition of the Oxidation State, *Pure Appl. Chem*. **88**(8), 831 – 839 (2016).

Richard G. Jones, Tatsuki Kitayama, Karl-Heinz Hellwich, Michael Hess, Aubrey D. Jenkins, Jaroslav Kahovec, Pavel Kratochvíl, Itaru Mita†, Werner Mormann, Christopher K. Ober, Stanisław Penczek, Robert F. T. Stepto†, Kevin Thurlow, Jiří Vohlídal, Edward S. Wilks, Source-based nomenclature for single-strand homopolymers and copolymers (IUPAC Recommendations 2016), *Pure Appl. Chem*. **88**(10 – 11), 1073 – 1100 (2016)

Lars Öhrström, Jan Reedijk, Names and symbols of the elements with atomic numbers 113, 115, 117 and 118 (IUPAC Recommendations 2016), *Pure Appl. Chem*. **88**(12), 1225 – 1229 (2016)

G. Michael Blackburn, Jacqueline Cherfils, Gerard P. Moss, Nigel G. J. Richards, Jonathan P. Waltho, Nicholas H. Williams, Alfred Wittinghofer, How to name atoms in phosphates, polyphosphates, their derivatives and mimics, and transition state analogues for enzyme-catalysed phosphoryl transfer reactions (IUPAC Recommendations 2016), *Pure Appl. Chem*. **89**(5), 653 – 675 (2017)

Jose Elguero, Is it possible to extend the Cahn-Ingold-Prelog priority rules to supramolecular structures and coordination compounds using lone pairs? *Chem. Int.* **38**(6), 30 – 31 (2016).

J. Reedijk, On the Naming of Recently Discovered Chemical Elements — the 2016 Experience, *Chem. Int.* **39**(2), 30 – 32 (2017).

R. Weir, IUPAC Standards and Recommendations, *Chem. Int.* **39**(2), 34 – 35 (2017).

R. Boucher, S. Heller, A. McNaught, The Status of the IUPAC InChI Chemical Structure Standard, *Chem. Int.* **39**(3), 47 (2017).