Risto Laitinen/August 4, 2016

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

Approved Minutes of Division Committee Meeting in Busan, Korea, 8–9 August, 2015

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 meeting for the first time. He described house rules and arrangements during the meeting.

KHH also regretfully reported that it has come to his attention that since the Bangor meeting in August 2014, Prof. Derek Horton **(**Member, Division VIII task groups on Carbohydrate and Flavonoids nomenclature; Associate Member, IUBMB-IUPAC Joint Commission on Biochemical Nomenclature) and Dr. Libuse Goebels, Member of the former Commission on Nomenclature of Organic Chemistry) have passed away. The meeting attendees paid a tribute to their memory by a moment of silence.

2. Attendance and apologies

Present: Karl-Heinz Hellwich (president, KHH) , Risto Laitinen (acting secretary, RSL), Richard Hartshorn (past-president, RMH), Michael Beckett (MAB), Alan Hutton (ATH), Gerry P. Moss (GPM), Michelle Rogers (MMR), Jiří Vohlídal (JV), Andrey Yerin (AY)

Observers: Leah McEwen (part time, chair of proposed project, LME), Elisabeth Mansfield (task group chair, EM), Johan Scheers (young observer, day 1; JS), Prof. Kazuyuki Tatsumi (past-president of the union, part of day 2)

Apologies: Ture Damhus (secretary, TD), Vefa Ahsen, Kirill Degtyarenko, Gernot Eller, Mohammed Abul Hashem, Phil Hodge (PH), Todd Lowary, József Nagy, Ebbe Nordlander (EN), Amélia Pilar Rauter (APR), Hinnerk Rey (HR), John Todd, Lidija Varga-Defterdarović.

3. Introduction of attendees

A short round of introductions was made.

4. Approval of agenda

Agenda was approved (Appendix 1).

5. Approval of minutes of meeting in Bangor, UK, 3–4 August 2014

KHH suggested several amendments to the draft minutes. In addition to noting several typographical errors and other technical corrections, he proposed significant modifications of the text in Sections 8.16.1 [*Source-based nomenclature of single-strand organic polymers (2003-042-1-800)*] and 8.17 [*End-of-line hyphenation of systematic chemical names (2014-003-2-800)*]. The minutes were approved with these amendments.

6. Matters arising

It was decided that the report given by AY in the Bangor meeting about recent extensions of the mol file format connected with InChIs should be included as an appendix to this year's minutes. AY promised to prepare the document (Appendix 2)

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

The contact persons for interdivisional information exchange, as decided in Bangor last year (see item 7 in the minutes of the Bangor meeting) and their reports on the interdivisional activity during the past year are as follows:

Division I. The assigned contact person is Andrey Yerin (Division I counterpart is Roberto Marquardt). He reported that there was no contact during the past year.

Division II. Assigned contact person is Alan Hutton (Division II counterpart is Daniel Rabinovich). However, during the past year there was virtually no contact between the divisions until Daniel Rabinovich attended the metallacycle task group meeting in Busan on August 7.

Division III. The assigned contact person is Amélia Pilar Rauter. There is no report of contact during the last year.

Division IV. Phil Hodge is the assigned contact person. Both PH and KHH are members of SPT providing natural overlap. There are several joint projects (see minutes 8.16 below).

The cross-over meetings were scheduled on Sunday Aug 9. There were two parallel session at 2 pm (Divisions II-VIII and III-VIII) and at 3 pm (Divisions IV-VIII and VII-VIII). It was decided to express in these meetings the need for more interaction. The Division Committee was represented in these meetings as follows:

Div. II-Div.VIII cross-over meeting: ATH, RMH, MAB, RSL
Div. III-Div. VIII cross-over meeting: KHH, MMR, AY, GPM
Div. IV-Div.VIII cross-over meeting: KHH, AY, JV, RSL
Div. VII-Div. VIII cross-over meeting: MAB, ATH, MMR

The minutes of the cross-over meetings are presented in Appendices 3-6.

TINCOPS task group (II-IV-VIII) will meet informally.

General discussion of the merits of the concept of preferred names and the desirability/feasibility of striving to establish such names in future projects.

TD has provided a discussion document (Appendix 7). He has raised the question, whether we should use PINs in inorganic chemistry. In the ensuing discussion, it was noted that apart from problems in creating inorganic PINs, it would be worthwhile to establish, how the chemical community has embraced PINs of organic compounds. The PIN project was started by the need of regulatory bodies to have one IUPAC name for organic compounds. It also indirectly led to the creation of Division VIII upon dissolving CNIC and CNOC at the end of 2001.

It was decided that now is a suitable time to have one or more workshops together with representatives of chemical industry to see, how much PINs are being used. A target could be to have joint meeting and possibly a joint project with the ACS nomenclature committee. MMR promised to explore the possibility with the ACS nomenclature committee to make a joint symposium (half a day) in the ACS National Meeting in San Diego. The follow-up could be that the Division Committee meeting next year takes place in Philadelphia in August 2016 in connection with the ACS fall meeting in which case there would also be a joint meeting with the ACS nomenclature committee. GPM promised to explore the possibility to organize a similar workshop/meeting with CICAG/RSC to evaluate the takeup and use of PINs for organic compounds. He reported later in the meeting that he had contacted Jeremy Frey of CICAG and received a positive reply. Organizational help would be worthcoming but getting funding might be difficult.

It was also decided that despite difficulties in creating PINs for inorganic compounds, the work on current PIN projects should still continue. ATH noted that one problem is to create a PIN for a complex, if the PIN of the organic ligand is not known. However, the methodology to construct a PIN can still be accomplished, even in cases where the organic ligand in a complex does not have a PIN.

8. Updates on Division VIII projects

8.1. IUPAC International Chemical Identifier (InChI) projects

There are several project concerned with InChI. The progress during the past year has been reported by Steve Heller (Appendix 8). The project on inorganic InChIs is not running. HR resigned from the subcommittee and Division. RMH has been asked to become the task group chairman but declined due to other commitments. Inorganic InChI is a world of its own and requires a specialist. The main objectives of the project is to find out, what information InChI should contain and how it should be presented. In this connection, there is a meeting of InChI Trust in Boston during the ACS National meeting in August 2015. RMH is member of InChI Trust.

RMH reported on the InChI Trust project for examining the development of the QR codes (2D bar code) version of the InChI. In this context RMH has initiated a project the objective of which is to identify and prioritise additional information to be included in the QR code in order to enhance their value and commercial utility (for example catalogue numbers, batch numbers, inventory

information, sample composition/purity, hazard codes and/or safety data URL) and it is being carried out by consultation with industry, regulatory bodies, and academia. Workshops will be organized in Busan on August 10, in Boston on August 19, and in Brussels in October. This project is complementary to another user-focused project that is developing InChI for mixtures.

LME reported on the proposal under review on InChIs for mixtures which is also focused on safety and hazard management as a use case. This project is intended to start in autumn. It was discussed whether InChIs are able to meet all required criteria, especially how they can deal with compounds in which the structure is only partially known, and how well they describe mixtures. AY noted that InChIs can handle mixtures, where all components are known, but it is more difficult, if there are unknown components in the mixture. RMH remarked that there is an InChI project concerned with reactions that should take care of this situation. KHH noted the analogous situation in polymers for which source-based names are available.

8.2. Preferred names in the nomenclature of organic compounds (the Blue Book) (2001-043-1-800)

KHH reported on the current status of the Blue Book revision, which has originated as a project aiming at preferred names for organic compounds. The project resulted in the complete revision of the Nomenclature of Organic Chemistry, which was published at the end of 2013. Since then numerous errors and inconsistences have been reported (GPM reminded the meeting that there is the URL http://www.chem.qmul.ac.uk/iupac/bibliog/BBerrors.html for the errata listing and an additional page for trivial textual and typographical errors). An email address bluebook@iupac.org has also been created for the collection of errors. Recently, however, the messages sent there do not come through. KHH will talk to the Secretariat. GPM assumed that most errors have probably been received by now.

The index of the Blue Book is insufficient. Further, the table of contents only extends to two levels of numbering, though more levels would be needed to render the table of contents useful. GPM has prepared such a detailed table of contents, which is under final revision and almost ready to be posted on the web.

According to the contract with RSC, the Blue Book can now be posted on the web in its entirety. The problem with the pdf, which is sold by RSC, is that it is produced as graphical images, which do not enable searches within the document. Furthermore, it would be ideal to be able to incorporate the corrections in the text before the pdf-version is published, but this is not allowed by the contract. Even if a searchable electronic version of the Blue Book becomes available, the inadvertent presence of extra spaces and other errors in the names need to be corrected to enable meaningful searches.

KHH stated that a project to revise the Blue Book is needed, because some inconsistences cannot be handled as errata. The objective is to get a new, corrected pdf edition. RSC, however, is not keen to allow corrections in the pdf. This problem needs to be discussed with with the Secretariat.

8.3. Nomenclature of cyclic peptides (2004-024-1-800)

GPM reported that though a document has been drafted a long time ago, there has recently been no progress. The project at topic 8.22, which is a subsection, has also seen no progress of that project.

GPM noted that while revision of the document (topic 8.3) is needed, it needs to be coordinated with the project covered under topic 8.22.

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

No progress since last year.

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

AY reported that a document is almost ready to be published. It covers four main methods describing the hydrogenation stages, for instance hydro-prefixes and indicated hydrogens.

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

GPM reported that there has been only little progress since last year, after Derek Horton passed away. He was the key person in the revision of the documents. There is still work to be done. A new document draft has just been circulated to the task group. KHH noted that the checking of the document against general nomenclature principles showed several errors and inconsistences that need to be corrected.

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

RMH reported that PINs for inorganic compounds have turned out to be problematic and little progress has been made during the past year. There are two key aspects that need to be developed for coordination compounds when designing PINs. The kappa convention needs to be extended and the principles of the selection of central atoms have to be specified. There is a disagreement about the multiplication of kappas along with the ligand. An exemption convention, when kappa is not multiplied along with the ligand has been proposed but has not met unanimous support among the task group members. The budget has run out and the task group has not met during the past year.

The central atom selection document is in its early stages. It is only after these two documents that the PIN question can be tackled (see also discussion in item 7).

[Secretary's comment: Those members of the task group, who were present in Busan, met briefly with some other members of the Division Committee after the end of the Division Committee meeting to consider the exemption convention and came to the conclusion that it should be dropped.]

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

RMH reported on the progress for the two Brief Guide-documents, which deal with condensation of inorganic and organic nomenclature (4 A4 pages each). The inorganic guide is complete and should be published in PAC in September. The publication took a long time and there were numerous

errors, which were caused by the change of the publisher during the processing of the manuscript. The organic guide is also coming along and will be published within the year.

In addition to PAC, the plan is that the 4-page documents will be published as centerfolds in CI. It is hoped that this centerfold will be made of somewhat thicker paper than what is normal in CI. It is also hoped that general inorganic textbooks would publish the guides as appendices, and they are also offered for publication in main chemistry journals. It was felt that a good dissemination plan is essential.

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

MAB reported on the activity of the borane task group during the past year After two meetings last autumn, a manuscript was prepared with the goal of having it published by the time of the Busan general assembly. There was a mini task group meeting in Busan to clarify the comparison of substitutive and additive nomenclature. While the document was not quite finished by the time of the Busan meeting, the final draft will be circulated soon and the project will end in being not too far behind the schedule.

8.10. Graphical representation standards for chemical reaction diagrams (2003-0045-3-800/2012-033-1-800)

KHH reported that there was only a little progress. The task group did not meet in Bangor due to lack of funds. Whereas two first parts have been published in 2006 and 2008, the part on reaction diagrams still needs to be completed. At the end of 2014, a new project proposal was made but not approved due to the absence of a formal progress report. The proposal therefore needs to be revised. KHH is prepared to make the application for extension. The size of the task group has to be reduced from the current size of 20 members to a maximum of ten members.

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

The activity of the task group on metallacycles was reported by ATH. Rapid progress has been made. There have been two meetings of the task group: London (January 29-30), Busan (August 7). The document is anticipated to be ready for review by the end of the year 2015.

8.12. Nomenclature of flavonoids (2009-018-2-800)

KHH reported that whereas quick resubmission of the manuscript to PAC had been hoped and APR had prepared the document, the progress was slowed down, because during the review, a list of flavonoid names was requested to be added as a table in the appendix. Furthermore, InChIs were also requested to be included in the document. These modifications increased the length of the document to over 100 pages. Since the additions also necessitate extensive checking, the finalisation of the project has been delayed.

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

KHH reported that this is a Division II project that is partly funded by Division VIII. There is no information of the progress. It was decided to discuss the current state of the project in the cross-over meeting.

8.14. Terminology and nomenclature of inorganic and coordination polymers (2011-035-1-800), abbreviated as TINCOPS

This is an ongoing project and will be discussed in the cross-over meeting (Dick Jones has had competing commitments of higher priority).

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

GPM reported that the project is based on a very old document. Whereas the existing molecules merit only short mention, new molecules need extensive treatment. The existing database should not be duplicated but important new information needs to be extracted.

8.16. Polymer projects (with Division IV)

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

KHH reported that after the Bangor meeting, a document was submitted for review. A few comments have been received. The sentiment of the comments was that polymer chemists want to retain names they have been used for decades. A new draft has been prepared, but the question remained, which traditional names should be retained. The selection of acceptable names was made in a joint meeting of the task groups of the preferred names for polymers and source-based nomenclature. The source-based document has been sent out to be refereed by Division VIII and SPT. Not many comments were received, and the document after another revision has been submitted to ICTNS.

8.16.2. Nomenclature and graphical representations for chemically modified polymers (1999-051-1-800/2006-006-1-800)

KHH reported that the document from this project was submitted to ICTNS last autumn and a number of comments have been received. Based on the comments, the revised version was prepared and was sent to public review, which lasted till the end of 2014. After further revisions, the manuscript was submitted for publication in PAC and was published as it was without further review and without page proofs. The final paper contained some 20 errors, several of which were introduced during typesetting. Errata have been published.

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

During the last year there have been several revisions of the document. JV noted that the last draft was distributed at the end of June. The document is close to be finished.

8.16.4. 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 reported that the document of preferred names for polymers is essentially a table of normally encountered constitutional repeating units (together ca. 250 constitutional units with systematic and acceptable, and no-longer recommended names). The latest document have had formatting problems and is thus delayed in its submission for review by Division VIII and SPT prior to review by ICTNS.

8.16.5. 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)

This project is on hold and is waiting for the preferred names for polymers. The final draft will be prepared by Phil Hodge. There is an online meeting with PH scheduled for August 10 to decide on the finalization of the document.

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

KHH reported that since the meeting last year there was no progress. The task group is going to have a meeting here in Busan during the SPT meeting next week.

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

KHH reported that the document for the guidelines for polymer abbreviations has been prepared and submitted for publication, but he did not see it prior to submission and it was published without the corrections made by KHH. *Angewandte Chemie* has prepared the German translation and asked KHH to correct the errors in the appendix as Supporting Information to the document. KHH did not consider this approach appropriate, since it might cause differences between the original publication and the translation. Therefore the *Angew. Chem.* publication waits for the final republication of the PAC publication.

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

KHH reported that the task group will meet in Busan on August 11.

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

This is a new project, which was discussed in Bangor. GPM and AY are on the task group because the expertise on organic and biochemical nomenclature is essential. The first meeting of the task group will be on August 12.

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

This project has seen a few drafts, for which RMH and KHH have given comments. It was noted, however, that in the revised version the comments of RMH have not been taken into account. RMH has sent his comments for the third time to the author. KHH remarked that he has not seen the latest version. GPM noted that hyphenation is a complicated process. The outcome depends on the

software, the author, and the publisher. It is essential that IUPAC should recommend how the software takes care of hyphenation.

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

EM reported that the project on nomenclature of carbon nanotubes and related structures met on August 7th, 2015 for discussions on the state of the project. As this project was initiated in conjunction with ISO TC 229 on Nanotechnology, the initial efforts of the group started with examining the ISO Technical Specification ISO/TS 80004-3 Nanotechnologies – Vocabulary – Part 3: Carbon nano-objects. It was decided prior to the meeting that the initial basic terminology will not be included, but the project would start with the terminology defined in Sections 3 and 4 of ISO/TS 80004-3. At the August 7 meeting, it was decided that the nomenclature will be modeled by the IUPAC fullerene and polymer nomenclature structures. Chirality was discussed, as the literature incorrectly uses a "chirality index" to indicate structure. In general, it was decided, the final recommendation will recommend that "chiral index" should now be called "a structural index", followed by a discussion of chirality. Details about how chirality would be applied to carbon nanotubes correctly will follow. A follow-up meeting is tentatively planned in conjunction with the Nanocarbon 2016 conference in Würzburg, Germany planned for February 23 – 24, 2015.

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

GPM had nothing to report, but hoped that there would be new information during the GA in Busan.

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

GPM reported that the task group had a meeting in November 2014. A document has been circulated in August 2015. The emphasis is in the enzymatic transfer reactions involving polyphosphates. The goal is to get numbering of individual atoms and to indicate prochirality.

8.21. Protecting groups abbreviations project (2011-044-1-300)

There is a published document with a few nomenclature errors, but there has been no new progress since the Bangor meeting. Depending on the nature and number of errors, there will be either an erratum or a new publication.

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

See Section 8.3.

9. Future projects/activities

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

There was a scoping meeting between Division VIII members and the representatives of ISO in London on January 28. A report on the meeting has been prepared by EN (Appendix 9):

Robin Macaluso is about to submit a project proposal on intermetallic phases, which is related to the nanoparticle project. The report on the scoping meeting will be sent to Prof Macaluso.

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

RMH noted that there are already new developments towards the new Red Book. For instance, solid state chemistry, which was not adequately covered in the 2005 RB, needs to be treated in the revised version. Polyhedral boranes, the revision of the kappa convention, the selection of central atoms, etc. also need to be covered in the future version of the Red Book. Principles of chemical nomenclature also contributes towards this new Red Book. RMH suggested that rather than updating the existing Red book, we should start from the clean slate. There is no need to start the project at this stage.

9.3. Graphical representation of polymers.

KHH reported that there has been no progress during the last year.

9.4. Rotaxane stereochemistry.

KHH reported that there has been no progress during the last year.

9.5. Delocalised systems.

AY noted that while some discussions have taken place during the last year, there is nothing new to report. There are problems in more complicated systems.

9.6. Crown nomenclature.

KHH reported that there has been no progress during the last year.

9.7. Central webpage for all IUPAC recommendations/publications.

KHH noted that we have to wait until the new IUPAC webpage is fully functioning (see item 13.3).

9.8. Document on italic and roman fonts.

KHH reported on the present stage of the document of roman and italic fonts: ICTNS was contacted for the need of an update. ICTNS initially concluded that there was no need for the update. The document on italic and roman fonts was, however, republished in issue 5 of CI (2015) in its original form, which contains numerous errors. ICTNS needs to be approached again to get this document revised and updated. Possibly we need our own project to make a usable draft. It was decided that either KHH contacts ICTNS or APR does. GPM will also convey the message to ICTNS in Busan. RMH indicated that it could be an ICTNS project and appear in PAC.

[Secretary's comment: KHH was in contact with ICTNS chairman, Ron Weir, and reported that the sentiment was that the publication of errata is sufficient. Since the actual document is short and the errors substantial, this errata is most likely a new document.]

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.

MMR noted that industrial compounds are often mixtures of species containing more than a single structure. They are traditionally named as single molecules, but this is often not sufficient for legal purposes. Furthermore, often these compounds are renamed several times, as the needs and situations change. RMH commented that if industry needs to name materials, they should consult a nomenclature specialist to solve the problem. It was decided that MMR will prepare an introductory document to underline the problem. It can then be decided whether there are grounds for a new project. RMH noted that this is pushing chemical nomenclature to new domains.

9.10. 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, ...).

TD has provided a discussion document (see Appendix 10). The document is concerned with a plethora of different, rather vague terms used in connection with various alternative names. The problem is illustrated by numerous examples. TD proposed that there is an urgent need to simplify this situation. In a general discussion it was considered that the term 'not acceptable' requires explanation. The terms "recommended" (could mean "preferred" or "acceptable"), "not acceptable", and "wrong" might suffice. ATH suggested that a document should possibly be prepared to define the appropriate terms to be used in nomenclature. MAB commented that there are two levels of terms. There are rules, which are applied in the construction of the name, but the name itself is a recommendation. It was decided to contact ICTNS to inquire how to proceed.

9.11. Other projects.

- Intermetallic solid phases. A task group has been formed by Robin Macaluso. The need to have somebody from the Division VIII committee in the task group will be evaluated, once the membership is known (see item 9.1).

- Class-name revision project (a joint project between Divisions VIII and III). KHH reported that the existing PAC paper is one of the most downloaded publications in PAC. There is still funding left for the project, but a new task group chairman and members have to be found. The project also needs to be approved by the end of the year.

- Supramolecular structures.

- Tautomers. AY will take the initiative.

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

KHH noted that the inorganic brief guide has its own e-mail address. The same needs to be done with the organic brief guide, once it is published.

11. Membership matters

11.1. Status of Division VIII Committee membership

A list each of the current Division Committee members and the proposed membership for the next biennium is given in Appendix 11. John Todd has resigned, therefore there is a vacancy for TM for 2016-2017. Michelle Monnens Rogers has been appointed in this position. Richard Hartshorn is a candidate for IUPAC Secretary General. If elected, there will be another opening. Gernot Eller is also willing to step down. According to the elections, the next two persons with most votes are Robin Macaluso and József Nagy.

There is a shortage of National Representatives. There are too few nominations and there might not be the full quota for the biennum 2016-2017.

[Secretary's note: In the meeting of the Council, RMH was elected Secretary General. Gernot Eller also indicated his willingness to downgrade his status from Titular Member to Associate Member. Therefore, after consulting them Robin Macaluso and József Nagy were appointed Titular Members for the biennum 2016-2017]

11.2. Division VIII representatives on other IUPAC bodies CCE, PAC Editorial Board, ICTNS, COCI, JCBN

CCE: RMH is willing to continue. The situation needs to be reconsidered, if he is elected Secretary General.
PAC Board: ATH
ICTNS: TD, if willing
COCI: MMR
JCBN: GPM (chair), KHH (ex officio), APR (AM), TD (AM)

11.3. Division VIII Advisory Subcommittee

The Advisory Subcommittee was set up to include persons who could be contacted on specific questions of nomenclature. The webboard (or discussion board) unfortunately does not work so that members of the Advisory Subcommittee cannot easily be contacted, and the list has not been updated on the IUPAC website. The contact details of the members also need to be updated.

ATH suggested that known Advisory Subcommittee members should be contacted by email and asked whether they are willing to continue in the advisory board. RSL will undertake this task.

12. Status on Division VIII web board with discussion forums

The web board is not working (see Item 11.3.).

13. Publicity

13.1. Division VIII (and related) publications since the 2014 Division Committee meeting

The publications that have appeared since the Bangor meeting are listed in Appendix 12.

There have been several presentations on different aspects of nomenclature by RMH (RSC), AY (ACS), and KHH (presentation in a school in connection with a chemistry olympiad winner). A more detailed list is presented in Appendix 13.

The Polish translation of the Blue Book is in progress. Requests for translations have also come from Japan.

Brief guides need to be circulated for instance in schools and general text books.

13.2. IUPAC-IUBMB nomenclature website

GPM has reported most recent events in connection with Blue Book errata. The errata list is very long and needs organisation. It also contains an extended list of contents (see Item 8.2).

[Secretary's note: It has been suggested that statistics of usage of the website should be minuted. However, no numerical data were mentioned in the meeting]

13.3. IUPAC website

Last year a project concerned with the redesign and renewal of the IUPAC website was initiated. There has been a task group evaluating the needs for improvement. At the end of last year, a contract was made to design a new website with the goal of having it running by the time of the Busan meeting. The schedule has been revised and the current goal is to complete the website together with the membership information by the beginning of 2016. The distribution of PAC and CI will also be managed via this website.

A demo version of the new webpage is running during the Busan meeting and will be demonstrated by Lynn Soby.

14. Reports from other IUPAC bodies

ICTNS: to be amended

[Secretary's note: Can we minute this? I have not received any information.]

JCBN: Meeting of JCBN was held in Braunschweig in May. The enzyme task force has long been the major project in IUBMB with the goal of building a database for enzymes. It will be an online

system and will enable all registered enzymes to be accessed freely. There was a working party meeting involving a brief discussion about flavonoids. A project concerned with small molecules is also being considered. (See also Items 8.3, 8.4, 8.6, 8.12, 8.15 above.)

CCE: RMH reported that there is a proposed joint project with CCE (see Item 15.1.)

15. Any other business

15.1. Visitor from Committee of Chemistry Education (Committee Secretary, Jan Apotheker).

The Secretary of CCE, Jan Apotheker, visited the Division Committee meeting. In the ensuing discussion it was concluded that the cooperation between Division VIII and CCE to form a joint project (nomenclature problems, new definition of the mole, measuring pH, etc.) is urgently needed. RMH noted that the trend in education should be to encourage critical thinking. Students need to be challenged. The Brief Guides could be used for education and they could act as source documents for translations to other languages. Brief Guides could also be used as source documents in text books, although there is a copyright problem: Brief Guides have to be taken in their entirety and reproduced unchanged.

There could also be YouTube-type clips to demonstrate the naming of the compounds, etc. ATH suggested that it could be worthwhile to develop a nomenclature app for tablets.

15.2. Strategic planning

RMH described the new IUPAC Strategic Plan, which will be up for approval during the Busan GA. The vision and mission have been redefined, core values added and short and long term objectives identified. The emphasis is on frequency of communication. Nomenclature will be at the core in promoting the international language of chemistry.

15.3. Miscellaneous Business

Cooperation with CCDC is needed. There could possibly be a meeting between the Division Committee and representatives of CCDC.

KHH has provided a report to the ACS Nomenclature Committee (Appendix 14). Although MMR will not be present in Boston ACS National Meeting, she promised to convey the report.

KHH has discussed with Ron Weir, the chair of ICTNS, the problems encountered when publishing in PAC.

16. Dates and venue for next meeting

The time and venue for the meeting of the following year was discussed. The main alternatives were:
(1) Istanbul (July 2016), (2) Philadelphia (August 2016), (3) Basel (August 2016), London (August 2016), Cambridge (August 2016).

17. Adjournment

KHH thanked everybody and adjourned the meeting.

APPENDIX 1

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

Agenda for Division Committee Meeting
Busan, Korea, 8–9 August, 2015

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 Bangor, UK, 3–4 August 2014

6. Matters arising

7. Interactions between Division VIII and other (IUPAC) bodies in relation to documents and projects involving chemical nomenclature.
General discussion of the merits of the concept of *preferred names* and the desirability/feasibility of striving to establish such names in future projects.

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

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

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

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

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

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

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

8.10. Graphical representation standards for chemical reaction diagrams (2003-0045-3-800/2012-033-1-800)

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

8.12. Nomenclature of flavonoids (2009-018-2-800)

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

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

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

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. Nomenclature and graphical representations for chemically modified polymers (1999-051-1-800/2006-006-1-800)

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

8.16.4. 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)

8.16.5. Revision of *IUPAC Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology* (2008-020-1-400)8.16.6. Definitions and notations relating to stereochemical aspects in polymer science (2009-047-1-400) (Web-based IUPAC recommendations on polymer nomenclature)

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

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

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

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 IUPAC Color Book Data Management (proposal 2013-052-1, Kinnan)
8.20 Nomenclature of Transition States and their Analogs for Phosphoryl Transfer Reactions (2013-039-2-300)

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

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

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.

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. 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, ...).

9.11. Other projects.

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

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. Status on Division VIII web board with discussion forums

13. Publicity

13.1. Division VIII (and related) publications since the 2014 Division Committee meeting

13.2. IUPAC-IUBMB nomenclature website

13.3. IUPAC website

14. Reports from other IUPAC bodies

ICTNS
JCBN
CCE

15. Any other business

16. Dates and venue for next meeting

17. Adjournment

APPENDIX 2

MOLfile format extensions for representation of chemical structures

So called **MDL MOLfile** is a simple text file format with extension *.mol serving for encoding of information about the atoms, bonds, connectivity and coordinates of a molecule. The MOLfile is sufficiently common that most, if not all, cheminformatics software applications are able to read the format, though not always to the same degree.

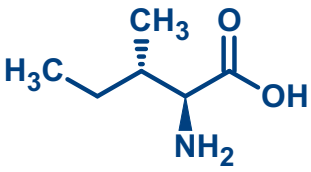
The format was created by MDL Information Systems (MDL) widely known for one of the oldest chemical drawing programs ISIS/Draw.

Now after several merges and acquires the official development of MOLfile belongs to BIOVIA.

(adapted from https://en.wikipedia.org/wiki/MDL_Information_Systems)

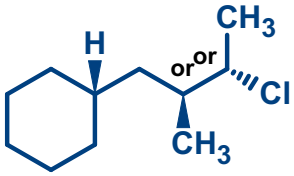
Thus, the MOLfile plays very important role in exchange of structural information between various chemical programs. While many other file formats exist and are used in chemistry related programs, the MOLfile is the most common and widely accepted.

The first paper describing MOLfile and related file formats appeared in 1992 - *J. Chem. Inf. Comput. Sci.*, **1992**, *32* (3), pp 244–255. The general principles of the format stayed unchanged for 20 years corresponding to MOLfile version V2000 and allowing definition of classical structures like the following:

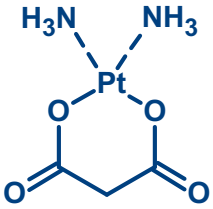


A possibility to define more advanced chemical objects with complex stereoconfiguration, haptic bonding and Markush substitution was introduced in MOLfile V3000. Before these enhancements such structures were depicted by means of graphic tools, like cycles and lines, or via vendor-specific tools without a possibility to exchange such objects between different applications.

The latest additions to MOL V3000 introduced in 2012 include hydrogen and coordination bonds, definition of multicenter haptic bonding and variable substitution for Markush structures. Now the following objects can be defined in chemically significant way allowing exchange in vendor neutral way.



Enhanced stereo – combination of absolute and relative configurations



Coordination of ammine ligands

Hapta-bonding in ferrocene

Markush structure defining three possible isomers

Note that some conventions of electronic representation may look not so obvious and lack endorsement via IUPAC or other recommendations, but such objects are long ago demanded and used by chemical science and industry allowing sensible encoding of the corresponding compounds.

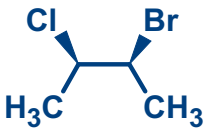
Many chemical drawing programs already support such representations, for example, BIOVIA Draw (Accelrys Draw), ChemDraw, ACD/ChemSketch and other. Several software vendors made available

freeware versions of the programs. For example, BIOVIA Draw can be downloaded free of charge for academic and personal use via the following link:
http://accelrys.com/products/collaborative-science/biovia-draw/draw-no-fee.php

Andrey Yerin
ACD/Labs, www.acdlabs.com
erin@acdlabs.ru

Appendix.

Examples of MOLfiles for the following structure



MOLfile V2000

```
  ACCLDraw07221612352D

  6  5  0  0  1  0  0  0  0  0999 V2000
    5.8003   -5.9391    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    6.1000   -5.4199    0.0000 Br  0  0  0  0  0  0  0  0  0  0  0  0
    6.1000   -6.4583    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.2008   -5.9391    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    4.9010   -6.4583    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.9010   -5.4199    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  1  0  0  0
  1  3  1  0  0  0  0
  1  4  1  0  0  0  0
  4  5  1  0  0  0  0
  4  6  1  1  0  0  0
M  END
```

MOLfile V3000*

```
  ACCLDraw07221612362D

  0  0  0     0  0            999 V3000
M  V30 BEGIN CTAB
M  V30 COUNTS 6 5 0 0 0
M  V30 BEGIN ATOM
M  V30 1 C 5.8003 -5.9391 0 0 CFG=1
M  V30 2 Br 6.1 -5.4199 0 0
M  V30 3 C 6.1 -6.4583 0 0
M  V30 4 C 5.2008 -5.9391 0 0 CFG=1
M  V30 5 C 4.901 -6.4583 0 0
M  V30 6 Cl 4.901 -5.4199 0 0
M  V30 END ATOM
M  V30 BEGIN BOND
M  V30 1 1 1 2 CFG=1
M  V30 2 1 1 3
```

```
M  V30 3 1 1 4
M  V30 4 1 4 5
M  V30 5 1 4 6 CFG=1
M  V30 END BOND
M  V30 BEGIN COLLECTION
M  V30 MDLV30/STEREL1 ATOMS=(2 4 1)
M  V30 END COLLECTION
M  V30 END CTAB
M  END
```

* V3000 MOLfile encodes the structure with relative configuration of stereocenters.

APPENDIX 3

Cross-over meeting of Divisions II and VIII

Attendees:

- Division II: Jan Reedijk (JR, The Netherlands), Lars Öhrström (LÖ, Sweden), Markku Leskelä (ML, Finland), Tiping Ding (TD, China), Ken Sakai (KS, Japan), Yang F. Abdul Aziz (YA, Malesia), Guillermo Ahumada (GA, Chile)
- Division VIII: Alan T. Hutton (ATH, South Africa), Richard M. Hartshorn (RMH, New Zealand), Risto S. Laitinen (RSL, Finland)

1. Organizational matters:

   a. There was some confusion in the relationship between the projects 2011-035-1-800 and 2011-028-1-200. It was concluded that there was a system error, since the number code and the title do not indicate that they are Division VIII projects.

   b. DR is a member of both boron and metallacycle task groups, but he couldn't participate because of the lack of Div. II funds. JR said that he needs to know well in advance with a proper request if funding is needed.

2. A report on InChI for inorganic compounds was presented in Istanbul. Since then there has been no progress. The task group leader has withdrawn from the project and a new task group chair is being searched.

   RMH reported that the descriptive character string of InChI is being converted to QR codes (analogous to the bar code but can be used as a link to web page). There is a possibility to include also additional information of the compounds, such as catalogue numbers, batch numbers, web pages, health and safety aspects etc. The chemical manufactures would place the QR code in the containers from where it can be read when needed.

   It is imperative to conduct a survey with users to establish what kind of information is needed. There will be a worksho during the General Assembly in Busan, and another one during the ACS National week in Boston. A third workshop was being planned to be held in Brussels by the end of the year 2015. RMH is the IUPAC representative in the InChI trust. ML noted that the EU chemical office in Helsinki should be interested in the development of InChI.

   It was also reported that a future project will be concerned with InChIs of mixtures. The funding will be provided by chemical companies or regulatory bodies.

3. Report of Division II:
   The following projects which were in preparing stage were presented
   a. The constitution of group 3 of the periodic table.
      In the project it is proposed that IUPAC should make an official recommendation in favor of the composition of group 3 of the periodic table as consisting either of
      (1) the elements Sc, Y, Lu and Lr, or
      (2) the elements Sc, Y, La and Ac.

b. Periodic Table of life
The aim in the project is to show via Periodic Table the importance and role of different elements to life

c. Survey of Definitions and Use of Common Solid-State Chemistry Terminology
Project's goal is to propose definitions of selected solid-state terms such as intermetallic, liquid crystal, semi-crystal, ionic crystal, molecular crystal, covalent crystal etc. None of these has an entry in the IUPAC Gold Book, a Google search of these terms reveals an acceptable definition for all of them.

d. Toward a comprehensive definition of valence
At present, term valence is used in connotations that imply several somewhat differing definitions. This project will research the history and current use of valence, analyze a series of examples, and consider whether a comprehensive definition of valence for atoms in compounds can be formulated.

4. Report of Div VIII:

a. TINCOPS: Document of inorganic single-strand polymers is 60 % ready. However, there are some interferences with the kappa rules that need to be sorted out.

b. Kappa (RMH): Draft document has been completed. The meeting of the task group appended by some other Division VIII members decided that the exemption convention will be removed from the document and the examples will be modified accordingly. TinCops can use the existing draft discrecarding the exemption convention. The concept of uncertainty-kappa is being debated and might be needed for single-strand polymers.

c. ATH reported that the Brief guide to inorganic chemistry (essentials in inorganic chemistry) has been published as an asap publication (no page numbers in PAC, yet). The four-page format is planned as an appendix. The PAC publication is in September and the future CI will have the four-page version as a centerfold. The analogous essentials of organic essentials is 80-90 % ready.

d. It was discussed how the use of chemical nomenclature nomenclature in wikipedia should be handled. There is a need to get the nomenclature information fixed in wikipedia without having random changes taking place. The copyright agreement of the Brief Guides allows the reproduction of the document in any format provided it is reproduced in its entirety and unchanged. One way is to have a reference with a hyperlink.

e. ATH described two projects in progress: A document on kappa-convention and that of the selection of central atoms. Div VIII is organizing workshops (ACS and RSC) to explore, how PINs are used by industry. In early 2015 there was also a scoping meeting between ISO/Div VIII on how to name nanoparticles. The role of Division II could be in the identification of suitable persons for such a project.

f. There is a need for a project for standardising the use of terms such as “acceptable”, “preferred”, “recommended”, etc. At the moment the terminology is confusing and does not assist clarity.

APPENDIX 4

Cross-over meeting of Divisions III and VIII

Attendees:

Division III: G. Michael Blackburn (GMB), Yi Jin (young observer), Ram Kandle (young observer)
Division VIII: Michelle Monnens Rogers (MMR), Karl-Heinz Hellwich (KHH), Andrey Yerin (AY)

- Division VIII Report (KH)
    - Blue Book – Appeared approx. 1½ years ago (Christmas 2013/New Year 2014)
        - Final production was pressed by IUPAC and publisher (Royal Society of Chemistry).
        - The publisher produced a subject index that was not expansive enough. The index also contains the long systematic names instead of the retained common names. Additionally, a number of standard prefixes were not found in the index. The errors in the index were addressed, but it was noted that these errors were also present in the main text which were also addressed.
        - Once the book was published, a number of errors and inconsistencies were noted and Division VIII began to collect and publish online a list of errata. Currently the list of errata consists of ca. 1000 entries. A procedure has been developed for committee members to review identified errata, and then - once checked by several Division VIII members - being put on the public list.
        - Division VIII is working on to develop a new version of the Blue Book that will hopefully be published as a PDF.
        - All findings of inconsistencies are welcome to be reported to bluebook@IUPAC.org.
    - Brief Guides of Nomenclature
        - Inorganic chemistry was just published at the end of July electronically in Pure and Applied Chemistry. It is expected to be printed in the September issue.
            - The 4 page formatted version will be a removable insert (centerfold) in Chemistry International.
            - The 4 pages formatted documents will also be the supplemental information on the Pure and Applied chemistry website.
            - Yi Jin recommended that the short guide be sent to book editors to assist them in reviews.
            - Division will send it to journal publishers to include in the author guidelines.
- Nomenclature at the interface of chemistry and Molecular Biology – Comment by GMB
    - Molecular biology has in some instances problems with use of accurate nomenclature and appropriate use of symbols.
    - Currently the president of International Union of Biochemistry and Molecular Biology (IUBMB) is Greg Petsko, who is a chemist. It would be recommended that an interaction be started with him to work to bring awareness of the appropriate nomenclature and symbols to the molecular biology community.
    - KH commented that through his work on the IUBMB-IUPAC Joint Commission on Biochemical Nomenclature (JCBN) he knows that this issue exists with molecular biology and partially relates to the fact that registered enzymes don't even change names even

when nomenclature evolves. While we have been successful in harmonizing, organic, inorganic and recently polymer nomenclature, changes to biochemical nomenclature and in molecular biology must be done carefully to bring acceptance.

- Division III Report
    - Nomenclature of ligands in transition states and their analogues for phosphoryl transfer reactions
        - Initiated based on interactions with crystallography, NMR spectroscopy
        - Over the past 20 years, there have been a series of trigonal bipyramidal and octahedral transition states and their analogues for phosphoryl transfer reactions. However, the issue is that there is no standard system for communicating the structure of these transition states within the field.
        - Historically within the crystallographic database they will name 2 different phosphate chains in the same molecule, one will be identified with letters and one with numbers.
            - A new systematic naming system is being developed to standardize how ligands will be named within structures.
        - The proposed nomenclature document is currently being reviewed.

- Joint project on updating the Glossary of Class Names should be initiated.

APPENDIX 5

Cross-over meeting of Divisions IV and VIII

Attendees:
Division IV: There were no introductions
Division VIII: Karl-Heinz Hellwich (KHH), Risto S. Laitinen (RSL), Jiří Vohíldahl (also Division IV, JV), Andrey Yerin (AY)

1. Report of Division VIII:

    a. TINCOPS: This is a joint project of the Divisions II, IV, and VIII. Document of inorganic single-strand polymers is 60 % ready. However, there are some interferences with the kappa rules that need to be sorted out.

    b. Kappa (RMH): Draft document has been completed. The meeting of the task group attended by some other Division VIII members decided that the exemption convention will be removed from the document and the examples will be modified accordingly. TinCops can use the existing draft disregarding the exemption convention. The concept of uncertainty-kappa is being debated and might be needed for single-strand polymers.

    c. KHH reported that the Brief Guide to Inorganic Chemistry (essentials of inorganic nomenclature) has been published as an asap publication (no page numbers in PAC, yet). The four-page format is planned as supporting information. The PAC publication is in September and the future CI will have the four-page version as a centerfold. The analogous document of organic essentials is 80-90 % ready.

2. The need of using systematic IUPAC nomenclature in naming solid-state phases was discussed. There is a need for a joint project or at least a representative from Division IV is needed to develop nomenclature for solid materials.
A new project on polymer microstructures was briefly mentioned.

3. It was proposed that Divisions IV and VIII interchange lists of members with 4 or 5 keywords concerning expertise of the members.

4. A potential concurrent meeting of Division IV and Division VIII Division Committees in Istanbul in 2016 was briefly mentioned, where it was stated that Division VIII would need organisational help from Division IV because Division VIII has no member from Turkey.

APPENDIX 6

Cross-over meeting of Divisions VII and VIII

Attendees:
Division VII: Schwenk, Cornelis, Johnston, Johannesen, Teh, Presley (guest), Uchiama (guest), young observer.
Division VIII: Richard M Hartshorn (RMH), Michael Beckett (MAB), Alan T. Hutton (ATH), Michelle M. Rogers (MMR)

- Division VIII
    - QR codes workshop for the International Chemical Identifier (InChI)
        - The InChI provides a way to encode molecular structure into a character string. There are multiple levels of data behind the InChI that includes stereochemistry, nomenclature, etc.
        - The InChI is looking to create a QR code for information related to a molecule
        - The workshop on Monday is to seek input from people on what additional information should be included in the QR code and to prioritize the possible additional information.
- Division VII
    - Synthetic cannabinoid drugs often will use common names in the papers instead of systematic names
        - They are looking for assistance in determining the systematic names
        - Assistance from Div VIII is offered (according to the possibilities in Div VIII)
        - If they are similar to base drugs, the base drug has an generated IUPAC name
        - RMH comments
            - that there can be several systematic names for a compound, however there is a project to identify Preferred IUPAC Name (PIN)
            - The software programs, ChemSketch and ChemDraw, are programmed to generate names based on the Blue Book, as they were programmed by Division VIII members. We would anticipate the names would reflect the nomenclature rules.
            - Recommend that Brandon get into contact with Gerry Moss for assistance with naming relating to this IUPAC project.
    - Nanoparticles
        - There was a meeting with ISO and Division VIII earlier this year to discuss a joint project on nanoparticles terminology
        - Currently there is nothing available to name inorganic nanoparticles however there is an ongoing project for carbon nanoparticles.
        - 2D nanostructures – what is the correct nomenclature. Is it correct to just add a –ene to the end?
            - RMH response – That is not nomenclature, that is terminology.
    - Medicinal and toxicology term glossary are often created by Division VII. Is there any process / mechanism to ensure that terms are not already defined
        - RMH comments:
            - ICTNS is responsible for ensuring consistency within IUPAC publications

- ICTNS is also responsible for the Gold Book. There is talk about possibly redoing the Gold Book

APPENDIX 7
Ture Damhus/July 31, 2015

Discussion paper for item 7 on the Division VIII Committee agenda for Busan, August 2015.

Item 7 reads
Interactions between Division VIII and other (IUPAC) bodies in relation to documents and projects involving chemical nomenclature.
General discussion of the merits of the concept of *preferred names* and the desirability/feasibility of striving to establish such names in future projects.

My main message is that we should put PINs projects on hold and think carefully about what the needs are and what is possible before we make any more promises or any further project proposals. And we should monitor in some organised way how the community reacts to the PINs published in the 2013 *Blue Book*.

Here are, somewhat unorganised, a few relevant thoughts about organic and inorganic PINs. I would only welcome comments and oppositional views.

1. In inorganic nomenclature, we are rather far behind organic nomenclature in terms of naming complex covalently bonded structures, in particular polynuclear coordination entities. It is rather obvious to me that providing a naming system at all for a lot more of these structures is more important or urgent than embarking on a project providing inorganic PINs. The work coming along with the kappa machinery and selection criteria for central atoms are of course (the) important elements in this endeavour. But whatever happens to boranes and nanoparticles in their respective projects, inorganic nomenclature at large also has to realise that there are clusters to name before we are done.

2. Organic PINs are about selecting names for drawn structures.*)
Once we are "done" with the coordination entities and perhaps the clusters (in our lifetime?), one could envisage carrying out a similar exercise as in the Blue Book for selecting inorganic PINs.
Questions arising are
- whether we would have any chance of succeeding, thinking of what goes on in the Blue Book
- whether there is a true need for a manual for selecting PINs for such fully specified complex inorganic structures.
See further under items 3, 4 and 5 below.

*) Almost true. I did incidentally see one PIN assigned to a structure not completely specified (P-68.3.1.3.3.1: the diazene oxide PIN at the bottom of p. 1009 does not specify where the oxygen atom sits on the N_2 group!). Other similar cases could easily be envisaged, and this does in principle create a bit of a problem. Is propanethioic acid a PIN for a mixture of tautomers? But these are just side remarks.

3. Concerns regarding PINs for fully specified structures based on experience with the 2013 Blue Book.
I may not be fair to the Blue Book in what comes here, but if my concerns are not justified, all the better.

What I experience as a user with probably more background than most people in the community (sorry to be immodest), but of course much less background and experience than the small group of persons who have worked intensively at writing and checking the book, is that the guidelines for generating PINs are mostly very local, and in many cases arbitrary choices are being made for single names or a few names. It is not a transparent overall system. As soon as one has a number of functional groups, or special functional groups, one has to look up rule after rule and it is not easy to maintain an overview and a feeling that everything is

consistent. Not many practitioners of chemistry are going to master those rules. Andrey Yerin would say the solution is to rely on good computer programs that generate names from structures. I am much more inclined to do that today than I would have been just a few years back. Still, the programs are created by humans, and the rules encoded (*i.e.*, the Blue Book rules) were also created by humans. Just like my own application of the rules will be subject to human error.

Just two quick examples of a beginner's uneasy feelings with the Blue Book.

Case 1. I hoped for general rules so looked up the rules for when I can use multiplicative nomenclature. From those rules I deduced that I can name the compound $H_2NNHC(=NH)NHNH_2$ as azanylidenemethylenedi(hydrazine).
In addition, criteria for multiplicative nomenclature to be senior to straight substitutive seemed to be fulfilled and I would have thought that I had the PIN.
Only if I recognise the exotic carboximidohydrazide group which is way down in Table 4.4, or if I stumble upon P-66.4.2.2, will I realize that the PIN is hydrazinecarboximidohydrazide. (The multiplicative name is not even mentioned there.)
However, replacing carbon by silicon, I would for sure be able to use the multiplicative name (for the probably very hypothetical compound obtained). Or if I replaced hydrazine by triazane, I don't think there is any functional group to interfere with my multiplicative name, so I suppose I would have the PIN correctly?
If all this is true, it is also true that the system is not easy to grasp and I get the feeling that I could well end up with a wrong name even when reading the rules carefully.
(Whether anybody except a few specialists will use a PIN like hydrazinecarboximidohydrazide is the kind of question we should seek to get answers for in 'customer surveys' of the PINs.)

Case 2. Another example: there are several places where names for EDTA are given in the Blue Book, but there is never a PIN. One of the places is in P-45.1.2. There is a rule there which to me is clear-cut: multiply the most numerous parent structure. For EDTA, two names can be constructed, one based on glycine (two occurrences of the parent) and one on acetic acid (four occurrences of the parent). Both these names are given in the second example in P-45.1.2. None is designated as the PIN, but an ordinary reader, I think, would assume that by chance the '(PIN)' designation had fallen away, as has happened in a number of other places, but that clearly the example was put there to illustrate the rule – and would conclude that the 'tetraacetic acid' name was the PIN.
(There has been a discussion in the Blue Book group some time ago in which it was concluded that there is no PIN for EDTA. I am not so sure. But if so, I have to say I do not understand the rule in P-45.1.2.)

4. For PINs for coordination entities with organic ligands, we need PINs for the ligands the way the whole thing is being built up at the moment. It is not good if there is no PIN for a common ligand like EDTA (see item 3 above) (yes, and partial and fully dehydronated forms thereof which may or may not be easier to deal with).

5. Most people in the community who might think of requesting inorganic PINs may not be primarily interested in PINs for fully specified complex structures (except perhaps for rare (?) cases like gadolinium complexes for magnetic resonance in medicine or the dinuclear manganese complex used as a bleach catalyst in automatic dishwash detergents...!).
The big market trades stuff like sodium silicates, sulfuric acid and sodium perborate tetrahydrate and will probably typically want compositional names. Nobody will appreciate dihydroxidodioxidosulfur for sulfuric acid. And the differences between 'sodium perborate tetrahydrate' and various more detailed coordination names of the tetrahydroxido-di-μ-peroxidodiborate type with or without kappas and charge numbers and renaming the compound as a hexahydrate may not necessarily be appreciated for customs purposes or environmental regulations.
But the problem with compositional names is that you will never be able to satisfy everyone, neither by overall rules or arbitrary conventions applied compound by compound. Is it iron(II) chloride or iron(2+) chloride or iron dichloride? What about calcium (di)chloride? Is it sodium sulfate or disodium sulfate? Is it aluminium trichloride or dialuminium hexachloride? Phosphorus pentaoxide? And so on.

6. In all fairness we should mention that we were exposed to substantial input from the real world and great sympathy for what we do in IUPAC at the customs chemists' conference in Brussels in 2011. Unfortunately, there was not much follow-up and personally I haven't had the time to review the material lately. But that contact is among several that should be taken up before trying to guess whether anybody out there seriously would use the PINs that we would be able to come up with for compounds of other than academic interest.

APPENDIX 8

InChI Trust Project Director's Report

July 2015 (07/14/15)

Summary:

Since the January 2015 report there continues to be good progress with InChI and the InChI Trust in a number of areas. I received the Patterson-Crane award for 2015 and will go to Columbus Ohio in September to accept the award and give an InChI presentation. The detailed technical paper on the InChI algorithm was finally published in the Journal of Chemoinformatics. Bio-Rad offered to rewrite parts of the InChI code to allow for threading (essentially parallel processing) so the algorithm would run faster. The US Patent Office, with help from the US NTIS (National Technical Information Service) has asked the Trust to participate in a workshop/seminar about InChI for Markush structures expected to be held the end of July. A new InChI working group on chemical mixture composition, which is related to lab safety, has been initiated. Related to the matter of the working groups, the main issue that, as usual, needs to be improved on is having the working groups be more active in moving towards their goals and getting more organizations, databases, and publications to use the InChI algorithm. Lastly Mark Ware has been engaged to write a briefing paper on InChI.

Items covered in this report:

Membership/Support:

Summary: A number of organizations are still in the process of joining or talking about joining, but there still is little progress in the past 6 months. 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 11, 2015

Existing Members and Associates: 14

Supporters: remains at 48

InChI RFP/Contracts

The contract for Markush structures with Digital Chemistry remains on hold awaiting potential funding. With the upcoming US Patent Office workshop/seminar on InChI for Markush structures perhaps this will be taken forward.

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. A RInChI working party meeting will be held during the Fall Boston ACS meeting to assess the progress and plan for future needs.

InChI development work

Igor Pletnev continues to do a superb and a very responsive job as the InChI programmer. What follows is a summary of his recent work:

"The new API has recently been analyzed and tested by Paul Thiessen of the NCBI/NLM/NIH. His uncensored comments are:

I really like this API. It's clean and straightforward. In retrospect, simpler to learn and use than the "native" API. I wrote an interface that directly translates PubChem's native format (a "PC-Compound" class object) to/from the IXA "molecule" – rather than, say, going through MOL/SDF. (Mostly I could copy this from the same interface I built for the regular InChI 1.04 stereo0d api.) I have run InChI generation, and conversely, generation of structure from InChI, across all of PubChem Compound. I did "round trips" – generating structure from InChI, then (re)generating InChI from that structure, to compare to the original InChI (and structure). I did not have any stability problems; no crashes/segfaults or anything like that.

Had to do some tweaking to get it to compile with GCC (4.8.1) on linux. Mostly type casts that GCC is kinda picky with. Had to replace memicmp with strncasecmp. Had to do a few small tweaks to compile all this within a unique C++ namespace – which I do so that, for example, I can build an application that uses both the IXA and the standard InChI 1.04 libraries simultaneously. (Which I needed to do to compare the two APIs side-by-side across all of PubChem.) Note that I do not have a standalone unix makefile for this library; the way I use it, it is compiled as a library into our NCBI C++ toolkit, and hence the Makefile configuration is embedded in that system, not useful outside that context. I did not compile a standalone application like inchi-1.

Fixed a substantial memory leak, by adding "FreeINCHI(&output);" to the end of BUILDER_Update() in ixa_builder.c.

It would be convenient to have MOL_GetBondOtherAtom() exposed in the public API.

Where I had to spend the most time was in figuring out how IXA's "stereo descriptors" work. The documentation on this was basically non-existent (unless I missed it, always possible). In particular, the array of atoms used as "vertices" in IXA are not (in general) the same as the atoms used as "neighbors" in the original library's stereo0D api. I actually had to read IXA code to figure out how these vertices are ordered and which atoms around the stereocenter they represent. So, it would of course be good to include in the documentation a complete discussion of how to create and read these stereo descriptors, and what it expects for each vertex atom. Graphical illustrations of how these vertices are arranged around the stereo atom/bond would be extremely helpful, rather than just text description.

When scanning across the entire PubChem compound database, results were basically identical for IXA vs 1.04 stereo0D.

There were a tiny number of cases (<1000 out of all 68M compounds) where IXA actually did better than 1.04, in generating structure from InChI. Mostly seemed to be cases of double bonds in a large (>6 atom) ring, e.g. CID 10059912. However, I can't swear for sure that this is a bug in the InChI 1.04 library, as opposed to a bug in my stereo0D->compound conversion.

I did not detect a single case where IXA failed but 1.04 succeeded.

Note that PubChem does not currently support allenic/cumulenic stereocenters, so I did not test that explicitly.

Overall, my impression of IXA is very positive. I would definitely recommend it being included in the "official" InChI code distribution."

Support of simple polymers.

This has been delayed due to numerous revisions in the InChI manuscript just published and is now expected to be finished in 2015.

IUPAC InChI subcommittee & working groups

IUPAC Committees

Chemical mixture composition

Leah McEwen at Cornell has initiated a working group for chemical mixture composition. Recent highly damaging events in chemical laboratories and classrooms [Sheharbano (Sheri) Sangji, a 23-year-old chemistry research assistant, died from injuries sustained in a chemical fire on December 29, 2008, in a laboratory at UCLA] 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

Positional Isomers

Considerable technical interest in positional isomers has developed in the past few months but at the same time Chris Steinbeck at EBI who had hoped to lead this effort has been promoted and does not have sufficient time to chair the working group. Chris is now looking for a new person to lead this working group.

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 – The work is now being done under Markus Sitzmann, with assistance from Evan Bolton at NIH/NLM/NCBI/PubChem. Markus continues to work on this – slowly. There is no new news to report

Polymers – This work was finished by the working group under Andrey Yerin. Igor has started programming this standard. The work will be completed and tested in 2015.

Reactions –With the August 2014 signing of a contract with Gerd Blanke this project is again moving ahead nicely. The RInChI working group will meet at the Boston ACS meeting to discuss the progress Gerd has made and what next steps are to be taken.

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: Grethe, Gunther

Members:
Colin Batchelor

Jonathan Goodman
Hans Kraut
Martin Schmidt
Keith Taylor

Markush – The US Patent Office, with help from the US NTIS (National Technical Information Service) has asked the Trust to participate in a workshop/seminar about InChI for Markush structures expected to be held the end of July 2015. Other than this there has been no progress as there is as yet no funding.

Electronic States – Don Burgess at NIST has developed plans for using InChI for Representations of Species at the Molecular Level. He has recently published the 3 papers on this subject about InChI-ER (Elementary Reactions). The last two came out in the June 2015 issue of IJCK. Being manuscripts from a US Government employee PDF copies are freely available from Don.

D. R. Burgess, Jr., J. A. Manion, and C. J. Hayes
International Journal of Chemical Kinetics **46**, 640-650 (2014)
Data Formats for Elementary Gas Phase Kinetics, Part 1: Unique Representations of Species at the Molecular Level
DOI: 10.1002/kin.20875

D. R. Burgess, Jr., J. A. Manion, and C. J. Hayes
International Journal of Chemical Kinetics **47**, 334-350 (2015)
Data Formats for Elementary Gas-Phase Kinetics: Part 2. Unique Representations of Reactions
DOI: 10.1002/kin.20912

D. R. Burgess, Jr., J. A. Manion, and C. J. Hayes
International Journal of Chemical Kinetics **47**, 361-378 (2015)
Data Formats for Elementary Gas-Phase Kinetics: Part 3: Reaction Classification
DOI: 10.1002/kin.20914

InChI for Materials – No news from the NIST staff about this.

Organometallics- Colin Batchelor and his working group expect a final report in late 2015.

Inorganics - The lack of a Chair for this working group has been an ongoing frustration. The current chair, Hinnerk Rey from Elsevier/Frankfurt, who replaced Nigel Wheatley, has had to resign owing to insufficient time available. This working group proposal to IUPAC for funding was approved in 2013 but there has not been any progress report yet.

2012-046-2-800: Handling of Inorganic compounds for InChI V2
http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2012-046-2-800

Chairman: TBD
Members:
Damhus, Ture
Druckenbrodt, Christian
Hartshorn, Richard
Schenk, Roger
Sitzmann, Markus

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

There will be a half-day session at the Boston CAS meeting chaired by Keith Taylor on this work. Nothing has happened since the October 2014 working group meeting at NIH.

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" was approved for funding by IUPAC. Marc will be holding a working group meeting on this at the Boston ACS meeting.

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) - Andrey Yerin will consider starting a project/working group (soon).

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. 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 prioritise 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."

Workshop Locations/Dates/Times

Workshop 1: Busan, South Korea, Monday 10 August, 17:00-19:00, coinciding with the IUPAC Congress and General Assembly

Workshop 2: Boston, USA, Wednesday 19 August, 17:00-19:00, coinciding with the Boston ACS meeting.

Workshop 3: Brussels, Belgium, details yet to be determined

January 2015 – July 2015 activities

Meetings Attended; Talks/Posters Presented

In April 2015 I attended the annual BioIT meeting in Boston. I met with and discussed InChI issues with a number of people at the meeting as well as having a meeting with Fabienne Meyers/IUPAC.

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, particularly Evan Bolton, to discuss InChI issues.

I met with Greg Banik, Bio-Rad, in June when I was in Philadelphia attending the BIO meeting. We discussed the offer from Bio-Rad to add threading capability to the InChI algorithm. At this time Greg is proceeding to undertake this work which will be thoroughly tested when delivered to the Trust for examination.

https://en.wikipedia.org/wiki/Thread_%28computing%29

https://en.wikipedia.org/wiki/Threaded_code

Manuscripts

The long overdue InChI technical manuscript was finally published in May 2015. The article "InChI, the IUPAC International Chemical Identifier" has now been published in **Journal of Cheminformatics, Volume 7, Issue 1** and is distributed with Open Access under the Creative Commons Attribution Noncommercial License.

The article is available electronically on SpringerLink:
http://www.springer.com/-/3/AU5bMkS9Khf9IB3kOfKX

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 a nice 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 – 728 (7/15); 629 views (12/14); 526 views (7/14)

The Googlable InChIKey – 915 views (7/15); 751 views (12/14); 597 views (7/14)

The Birth of the InChI - 984 views (7/15); 835 views (12/14); 687 views (7/14)

What on earth is InChI? - 2,956 (7/15); 2486 views (12/14); 1977 views (7/14)

An update on the Open Source InChI project – 1,702 views (7/15)
https://www.youtube.com/watch?v=F9XppyZg4E4

IUPAC InChI – 922 views (7/15)
https://www.youtube.com/watch?v=mH9fuspg_h0

Representing Chemical Structures on computer – 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 – 354 views (7/15)

https://www.youtube.com/watch?v=V9HHnRAS5BA

Two other YouTube InChI videos are available:

Mcule video:
2012 San Diego ACS presentation: Registration system of mcule: InChI is the key
128 views (7/15); 122 Views (12/14 – uploaded 2012)

Audiopedia video
International Chemical Identifier
29 views (7/15) 5 views (12/14 – uploaded 11/14)
(1 minutes video):
http://youtu.be/MG49gn_CdUE

Published on/Uploaded to YouTube Nov 30, 2014:

"The IUPAC International Chemical Identifier (InChI /ˈɪntʃiː/ IN-chee or /ˈɪŋkiː/ ING-kee) is a textual identifier for chemical substances, designed to provide a standard and human-readable way to encode molecular information and to facilitate the search for such information in databases and on the web. Initially developed by IUPAC and NIST during 2000–2005, the format and algorithms are non-proprietary. The continuing development of the standard has been supported since 2010 by the not-for-profit InChI Trust, of which IUPAC is a member. The current version is 1.04 and was released in September 2011.
Prior to 1.04, the software was freely available under the open source LGPL license, but it now uses a custom license called IUPAC-InChI Trust License."

Technical Issues

The mechanism to discuss and resolve technical issues continues to work well. 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 for the second half of 2015

For 2015 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. Attend ACS meeting in Boston and meet with groups to discuss adoption and usage of InChI.
4. Attend the GDCh Fulda meeting and present there.
5. Attend the Pacifichem meeting and present a poster and co-author a talk on InChI for Health & Safety data.

Steve Heller

APPENDIX 9

Report on scoping meeting between IUPAC (Division VIII) and ISO regarding nomenclature/terminology of inorganic nanoparticles

Participants

IUPAC (representatives of Division VIII): Ebbe Nordlander, Risto Laitinen, Alan Hutton, Edwin Constable, Jeffery Leigh, Michael Beckett

ISO: Yasir Sultan, Eric Gulliver

On Jan 27 and 28, 2015, a scoping meeting was held in London, UK, between representatives of the International Organization for Standardization (ISO) and IUPAC. The task was to investigate the possibility of a joint project between the two organizations on the terminology and nomenclature of inorganic nanoparticles (excluding carbon-based nanoparticles) and terminology for inorganic nanoparticle-based conjugates. Representatives of ISO described the current needs in this area, and the efforts that have already been made in the nomenclature/terminology area regarding the above-mentioned problem. Both regulatory agencies and industry, and to a lesser extent, front-line researchers, have an established need for the definition and development of nomenclature for (polydisperse, but reasonably uniform) nanoparticles. Such nanoparticles need to be defined in terms of (i) core composition and "structure" (the latter not always being absolute, or clearly definable) (ii) possible surface coverage and modification (nature of surface layer, both in terms of constituent molecules/substances and layer properties/dimensions) (iii) morphology, including structure of metal particle surfaces, and (iv) physical properties of the nanoparticles.

The ISO and IUPAC representatives realized that because of the inherent "vagueness" of the identities of nanoparticles, new nomenclature that is not merely an adaptation of existing IUPAC nomenclature must be developed. An extension of present IUPAC nomenclature to include systematic nomenclature of metal clusters will not be sufficient to meet the needs of the nanoparticle scientific and regulatory community. A joint working group addressing items (i) and (ii) above needs to be established. An IUPAC project to initiate the development of such nomenclature should be launched, with the goal of producing a Technical Report. Such a Technical Report may form the basis for further study towards IUPAC recommendations, and it is realized that any further development will likely require the involvement of regulatory and legislative bodies (ECHA, FDA etc.). Furthermore, because of the nature of the problem(s), consultation with IUPAC Division II (Inorganic Chemistry) and ICTNS is required. Finally, realization of objective (ii) will most likely require involvement of participants with expertise in surfactant and/or polymer chemistry. External consultation with professional and regulatory bodies representing material science and physics is essential.

None of the IUPAC representatives present at the scoping meeting possesses the expertise required to lead the envisaged IUPAC project. Such a project leader should have experience in materials science, and the chemistry of nanoparticles, as well as experience of and/or interest in nomenclature. The identification of such a project leader

will be critical to the success of the project. It is, however, important that the project incorporates

several members of IUPAC division VIII (Nomenclature) to ensure liaison with the division and proper integration and compliance with existing IUPAC nomenclature projects and recommendations.

The scoping party suggests that a possible starting point for the development of the envisaged nomenclature/terminology should be treatment of metal core (including mixed metal core) nanoparticles with surface coverage and modification. Metal-chalcogenide cores should not be included in the initial efforts. Furthermore, the scoping party suggests that a further interdivisional meeting to discuss a potential joint ISO/IUPAC project should be held in conjunction with the IUPAC General Assembly in Busan, South Korea. Such a meeting should include at least one ISO representative, who may need funding for his/her participation.

Discussions within the scoping party and, in particular, with the representatives of ISO established that this initiative represented a fundamental new opportunity for IUPAC. The emphasis of the efforts in nomenclature to date has been in the precise nomenclature of discrete and monodispersed molecular systems. The extension to nanomaterials raises three distinct issues that challenge the existing expertise within IUPAC (i) the move from monodispersed to polydispersed systems (ii) the complexity of the nomenclature required predicates hierarchical levels of description and (iii) multiple components are likely to be present in non-stoichiometric and variable ratios. IUPAC has some experience with the first issue with respect to the nomenclature of polymers and the scoping group recommend consultation with this panel of experts as well as experts in the use of fuzzy logic to define such problems. For the second issue, the group considers that InChI descriptors provide the best starting point, in particular with the mid-term wish of ISO to develop bar-codeable systems. The third issue is well within the competencies and experience of IUPAC to solve, in particular, in combination with InChI coding.

Furthermore, the possibility of developing (the) nomenclature for metal clusters was discussed. Although such nomenclature is not applicable to nanoparticle nomenclature per se, it was realized that there is a need for such nomenclature within the chemistry community, and that this problem has not been adequately addressed by present nomenclature efforts. The participants at the meeting agreed that any extension of current nomenclature to cover larger clusters will rapidly lead to the generation of names that will be very long and impracticable, and will therefore not be used. It is recommended that the nomenclature for such clusters will instead be InChI nomenclature. Such nomenclature will be unambiguous and easy to codify, and will therefore be amenable to database usage. The key problem will then be that of designing and developing an IUPAC structure convention for clusters, with a set of rules for assigning numbers/identifiers to all cluster atoms. Efforts have already been made to tackle this problem, but the solutions that have been presented do not yet cover all possible structures. The working party suggests that a potential project to develop InChI-based cluster nomenclature is discussed at the IUPAC General Assembly in Busan, South Korea, together with representatives of the InChI developers and the InChI trust.

APPENDIX 10

Ture Damhus/July 31, 2015

Discussion paper for item 9.10 on the Division VIII Committeee agenda for Busan, August 2015.

Item 9.10 reads

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, ...).

Discussion

I claim that
- Users of IUPAC's nomenclature publications will typically just want to know what is an acceptable name and not be interested in *degrees* of acceptability.
- Some users may be interested in *arguments* for IUPAC accepting one or the other name or not accepting some names (the latter in particular if IUPAC does not accept a name they have been using themselves).
- Some users may request a single acceptable name, *i.e.*, they will be interested in PINs (provided the PINs fulfill whatever requirements these users may have for the names they need).

If the above description of the situation in the community is basically correct, IUPAC nomenclature publications should only use the terms 'acceptable', 'not acceptable' and 'preferred' (or some equivalent set of terms, explicitly defined – it is not the exact words chosen that is my point here).

However, this has by far not happened in recent publications.

Samples follow of language found in recent IUPAC nomenclature publications (all of which are by the way entitled **Recommendations** rather than **Rules** as used in earlier times).
Many of the terms used appear in several publications but may be exemplified here only from one of them. Unless otherwise stated, boldfacing is mine, to highlight the terms I am focusing on. References of the types 'I-', 'R-', 'IR-' and 'P-' refer to sections in the 1990 *Red Book*, the 1993 *Blue Guide*, the 2005 *Red Book*, and the 2013 *Blue Book*, respectively. Other sources are stated explicitly.

'names **recognised** by IUPAC' [*Principles* 2.4]
'

...for example 'borata'...**no longer recognized**' [2013 *Blue Book* p. xxix]

(TD: there are several meanings of the word recognise in daily life, and the immediate question will be whether 'recognised' is the same as acceptable.)

'(nomenclature) methods **allowed** by IUPAC' [*Principles* 2.4]

(TD: one could mistakenly think this has something to do with law! I don't say this for fun – for some users, 'IUPAC names' are tied to laws and regulations.)

'some **traditional trivial names** are **still allowed** [*Principles* 5.4; but in *Principles* 4.1 it says: 'trivial' is not dismissive or pejorative]

'**should no longer ever be used**' (about 'ous'/'ic' endings for designating oxidation states) [*Principles* 5.4] – but later in 5.4: 'ous'/'ic' is **no longer recommended** for element cations

'IUPAC does **not approve** (about designating charges with repeated plus or minus signs)' [*Principles* 5.4]

'sulfonium is **no longer recommended**, oxonium is **still acceptable**' [*Principles* 5.5]

'NO^{2+} was **formerly called** the nitryl cation, but it is **now named** dioxidonitrogen(1+)' [*Principles* 5.5]

'an **equally satisfactory name**', 'could **equally be named**' [*Principles* 5.6.3]

'**retained for present use**' [*Principles* 6.5]

' (the Red Book 2005) **advises** that 'hydrido' **would be preferable in such circumstances**' (followed by examples with names given as '...hydro...' **or** '...hydrido...') [*Principles* 10.1.2]

'...have now been **abandoned**...' [IR-1.6.7]

'...**correct names**...' [IR-1.6.4]

'...carbonohydrazide **preferred to** carbohydrazide and carbazide' [*Blue Guide* Table 31]
(TD: so what about the two latter names)

'...sulfanyl is **preferred to** mercapto which was **used in previous editions**' [*Blue Guide* Table 5]; '...mercapto .,. **not included in these recommendations**' [R-5.5.2]

'...methylthio... **not encouraged in these recommendations**' [R-0.2.3.3.8, footnote 9]

'this method is not continued in these recommendations' [R-2.4.4.1, footnote 34]

'...has been **used traditionally and** is **still to be preferred in these recommendations**' [R-3.1.3]

'**traditionally** azomethane' [R-5.3.3.1; but in footnote 60 designated as 'an acceptable alternative']

'...thiocarbaldehyde **has been used in the literature**...' [R-5.6.1]

'...the contracted form benzaldoxime **has been used**' [R-5.6.6.1, footnote 80]

'*Note:* ...ethylene oxide ... **has also been used**' [R-5.3.3.1]
(TD: and so was it acceptable in *Blue Guide*? Neither oxirane nor epoxyethane is explicitly mentioned. Because the language is vague in the note and the preceding paragraph giving the general methods is rather involved, the careless reader may well have gone away with the impression that "the IUPAC name" was ethylene oxide.

For some users, this may have been reinforced by reading the 2008 *Purple Book* 11.2, where poly(ethylene oxide) is classified under 'semisystematic or trivial source-based names' that are '**approved for use in scientific work**' (!!), indicating that ethylene oxide is acceptable [but see the oncoming publication on source-based polymer nomenclature].
In the 2013 *Blue Book*, we have oxirane (PIN) and ethene oxide, but are still left in uncertainty regarding epoxyethane, which should be acceptable in general nomenclature as formed by method (4) there, but is not listed in the example together with the other two names. However, that is not a problem of the language used.)

'...**formerly** furazan' (about 1,2,5-oxadiazole) [R-2.3.3.1]

'the prefix 'guanidino' is **no longer acceptable in preferred IUPAC names**' [*Blue Book* p. xxxii]; ...the prefix guanidino is **no longer recommended'**; '...the prefix guanidino is **no longer acceptable in IUPAC nomenclature**' [P-66.4.1.2.1.3]; and later, '...***the* systematic name** for arginine is 2-amino-4-carbamimidamidopentanoic acid' (my italicisation; but the preferred prefix is carbamimidoylamino) [P-103.1.1.1]
(TD: 'no longer acceptable in preferred IUPAC names' does not make sense; previously there *were* no preferred IUPAC names)

'...'fulminate' ... **discarded** in favor of systematic names' [*Blue Book* p. xxxiii]

'...**deprecated** names...' [P-62.2.2.1]
(TD: Currently there is a discussion about an upcoming publication, where the task group leader wishes to use the word 'deprecated' to 'express distaste' for the name in question. I maintain that expression of distaste does not belong in our publications and that users will wonder whether different behaviour is expected from them regarding deprecated names versus other not acceptable names that are not given this extra "qualification".)

'...alkyl glycosides receive also functional class names that are **classified as approved names in carbohydrate nomenclature**' [P-15.2.1.1]

'...sulfamide....**discouraged**, although ... importance in medicinal chemistry is well established' [I-9.5.3.5]

'....formazan **can also be named** substitutively' [P-68.3.1.3.5]
(TD: presumably meaning that a correctly constructed substitutive name will also be acceptable....)

P-68.3.1.2.6.1: hydrazinecarbohydrazide (PIN) is shown with one set of locants, but '**also recommended**' is carbonic dihydrazide with another set of locants (but 'only for general nomenclature')

'***The* IUPAC name** is bis(chloromethyl)aminoxyl' [Gold Book under 'nitroxides'; my italicisation]

Special note 1: In some publications, certain names are listed with the word 'not' (sometimes boldfaced in the publications) in front of them, e.g. '**not** thiophenol' [R-5.5.1.2].

Blue Book 2013 explains in P-60.2 that 'not' is used when the name following it is '**incorrect**', taken to mean that it is **constructed not according to the rules** being presented. There are clearcut uses of 'not' in this way also earlier in the book (*e.g.*, in connection with the '**correct**' and '**incorrect**' spiro names given in examples in P-24.2.2.1).
However, in other cases, it is used more broadly, *e.g.*, when exemplifying that a not (fully) systematic name has now been classified as not acceptable for whatever reason. *E.g.*, in P-68.3.1.4.1: 'not 5-(hydroxymethyl)furfural'. The reason here is not that the general systematics is wrong, but that it has been decided arbitrarily that substitution in furfural is not acceptable now.

In P-21.2.3.1, the use of 'not' is stretched rather far where it says 'not disilazane'. The text above says that amine names (*in casu N*-silylsilan-1-amine) are preferred (must be understood to mean: when constructing (preferred) IUPAC names for organic derivatives); it does not say, and cannot say, that the inorganic name – which is formed according to *Red Book* 2005 – is not acceptable *per se*. But that is what the user browsing for examples rather that reading the text will think.

Special note 2: It is of course particularly problematic when different places in the same publication or in parallel IUPAC publications are or seem to be contradictory or inconsistent. If language is slightly different in such cases, the user may become even more in doubt about the exact meaning of the various expressions.

Examples of this are:

'phosphine is no longer recommended, phosphane being preferred' [*Principles* 6.2.10]; 'phosphine, arsine, stibine no longer acceptable' [Table IR-6.1]; 'phosphine, arsine, stibine retained for use in general nomenclature' [P-21.1.1.2]

'phosphorane, arsorane, sulfurane, ... not recommended – the λ convention is preferred' [I-7.2.2.1]; 'phosphorane, arsorane, stiborane retained for use in general nomenclature; sulfurane not recommended' [P-21.1.2.1]

'names such as trithiocarbonic acid are not recommended' [I-9.5.2.1]; 'trithiocarbonic acid' given as example of the use of prefix 'thio' [R-5.7.1.3.4]

The two publications in 2006 and 2008 on graphical representation standards attempted to be strict in terminology by only using the terms 'preferrred', 'acceptable', 'not acceptable' and 'wrong'. However, in the discussion of these terms there is still some vague language: 'not acceptable' is said to mean that the representations in question '**should be strongly avoided in normal usage**' but at the same time **'are not acceptable under any circumstances**'.

I find it necessary to clean up this jungle of terms. It is not acceptable that IUPAC, supposedly taking responsibility for chemical terminology in addition to chemical nomenclature, cannot decide on a strict and consistent vocabulary in its nomenclature recommendations.

It can well be that 'recommendation' is in fact to the point and that 'recommended', or at least 'not recommended' (or perhaps 'approved' and 'not approved'), should supplant other terms highlighted above. I leave that to oncoming discussions. But, I strongly recommend (!) that we end up having only two categories: names we (= IUPAC) think it is acceptable to use, and names we think are not acceptable. Certain names in the first category will be PINs (a subcategory).
Everything else we feel like expressing ourselves about – history of names, current or past usage, reasons for keeping names in their category or moving them from one category to the other, *etc.* – is background material and should clearly be kept apart as such.

Appendix 11

Division VIII Membership 2014-2015

Name	Status	Term	NAO
Dr. Karl-Heinz Hellwich	TM-President	2014-2017	Germany
Dr. Ture Damhus	TM-Secretary	2012-2015	Denmark
Dr. Richard M. Hartshorn	TM-Past President	2014-2015	New Zealand
Dr. Michael A. Beckett	TM	2014-2015	United Kingdom
Prof. Philip Hodge	TM	2014-2015	United Kingdom
Prof. Alan T. Hutton	TM	2014-2015	South Africa
Prof. Risto Laitinen	TM	2014-2015	Finland
Prof. Ebbe Nordlander	TM	2014-2015	Sweden
Prof. Amélia Pilar Rauter	TM	2014-2015	Portugal
Dr. Hinnerk Rey	TM	2014-2015	Germany
Dr. Kirill Degtyarenko	AM	2014-2015	Spain
Prof. Mohammed Abul Hashem	AM	2014-2015	Bangladesh
Dr. Michelle Monnens Rogers	AM	2014-2015	United States
Dr. John B. Todd	AM	2014-2015	United States
Prof. Jiří Vohlídal	AM	2014-2015	Czech Republic
Dr. Andrey Yerin	AM	2014-2015	Russia
Prof. Vefa Ahsen	NR	2014-2015	Turkey
Prof. Dong Joon Choo	NR	2014-2015	Korea
Dr. Gernot Eller	NR	2014-2015	Austria
Prof. Wei Huang	NR	2014-2015	China
Prof. Todd L. Lowary	NR	2014-2015	Canada
Prof. József Nagy	NR	2014-2015	Hungary
Prof. Martin Putala	NR	2014-2015	Slovakia
Mrs. Sumalee Tangpitayakul	NR	2014-2015	Thailand
Prof. Lidija Varga-Defterdarović	NR	2014-2015	Croatia
	NR	2014-2015	
Dr. Gerard P. Moss	*Ex Officio*	2014-2015	United Kingdom
	10 TMs, 6 AMs, 9 NRs		

Proposed Division VIII Membership 2016-2017

Name	Proposed Status	Proposed 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
Dr. Gernot A. Eller	TM	2016-2017	Austria
Prof. Richard M. Hartshorn	TM	2016-2017	New Zealand
Prof. Philip Hodge	TM	2016-2017	United Kingdom
Dr. John B. Todd	TM	2016-2017	USA
Prof. Jiří Vohlídal	TM	2016-2017	Czech Republic
Dr. Michael A. Beckett	AM	2016-2017	United Kingdom
Prof. Ivan L. Dukov	AM	2016-2017	Bulgaria
Prof. Robin Macaluso	AM	2016-2017	USA
Prof. József Nagy	AM	2016-2017	Hungary
Dr. Michelle Monnens Rogers	AM	2016-2017	USA
Dr. Keith T. Taylor	AM	2016-2017	USA
Dr. Fabio Aricó	NR	2016-2017	Italy
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
	NR	2016-2017	
	NR	2016-2017	
Dr. Gerard P. Moss	*Ex Officio*	2016-2017	United Kingdom
	10 TMs, 6 AMs, 6 - 8 NRs		

Appendix 12

Publications that have appeared since the Bangor meeting (August 2014)

R. G. Jones, T. Kitayama, E. S. Wilks, R. B. Fox, A. Fradet, K.-H. Hellwich, M. Hess, P. Hodge, K. Horie, J. Kahovec, P. Kratochvíl, P. Kubisa, E. Maréchal, W. Mormann, C. K. Ober, R. F. T. Stepto, M. Vert, J. Vohlídal, Nomenclature and graphic representations for chemically modified polymers (IUPAC Recommendations 2014), *Pure Appl. Chem*. **87**(3), 307 – 319 (2015); Erratum: *Pure Appl. Chem*. **87**(4), 441 (2015).

R. M. Hartshorn, K.-H. Hellwich, A. Yerin, T. Damhus, A. T. Hutton, Brief Guide to the Nomenclature of Inorganic Chemistry *Pure Appl. Chem*. **87**(X), xxx – yyy (2015); DOI: 10.1515/pac-2014-0718 (currently available online as ASAP publication).

I. Mills, On the Use of Italic and Roman Fonts for Symbols in Scientific Text, *Chem. Int.* **36**(5), 23 – 24 (2014).

Mark I. Borkum, Jeremy G. Frey, What's in a Name? Quite a Lot, as it Happens! *Chem. Int.* **37**(2), 7 – 9 (2015).

Evan Hepler-Smith, The History of the IUPAC Nomenclature of Organic Chemistry, *Chem. Int.* **37**(2), 10 – 14 (2015).

German translations of IUPAC-Publications (2014 – 2015)

The journal *Angewandte Chemie* (*Angew. Chem*.) has since 2002 been publishing translations of IUPAC Recommendations and Technical Reports into German.

32 translations were published from 2002 through 2010, one revised translation in 2011, and three further translations have been published in 2014.

In addition, the publication of a translation of the Abbreviations of Polymer Names and Guidelines for Abbreviating Polymer Names (IUPAC Recommendations 2014) [*Pure Appl. Chem.* **86**(6), 1003 – 1015 (2014)] is intended. The document has been translated and KHH was asked to check the translation and whether he would be able to provide the corrections to the Appendix which will only be reproduced as Supporting Information. After having talked with the responsible editor she decided to put the translation on a hold until a corrected republication of the original publication in order to avoid inconsistencies between the English and the German document.

Carsten Schmuck*, Juliane Keilitz
Glossar von Begriffen zur Assoziatbildung und Selbstorganisation in den Polymerwissenschaften *Angew. Chem.* **2014**, *126, Nr. 11*, 3078 – 3091

Original: **Pure Appl. Chem.** *85*, 463 – 492 (2013)

Carsten Schmuck*, Elisabeth Weber
Definition der Halogenbrücke
Angew. Chem. **2014**, *126, Nr. 24*, 6391 – 6392
Original: **Pure Appl. Chem.** *85*, 1711 – 1713 (2013)

Roland A. Fischer*, Inke Schwedler
Terminologie von Metall-organischen Gerüstverbindungen und Koordinationspolymeren
Angew. Chem. **2014**, *126, Nr. 27*, 7209 – 7214
Original: **Pure Appl. Chem.** *85*, 1715 – 1724 (2013)

APPENDIX 13

Presentations of Nomenclature

Hartshorn, R.M. (2014) What's In a Name? Possibly Death and Taxes! Royal Society of Chemistry, London, UK: RSC Chemical Information and Computer Applications Group Meeting, 21 Oct 2014.

Presentations by KHH and AY.

APPENDIX 14

Dr. Karl-Heinz Hellwich
Postfach 10 07 31
63007 Offenbach
Germany
Phone: xx49/6041/9621785
Phone (office): xx49/69/716731-23 (Tue - Fri)

International Union
of Pure and Applied
Chemistry

Division of Chemical Nomenclature
and Structure Representation

July 31, 2015

Report to ACS Nomenclature, Terminology, and Symbols Committee

It is my pleasure to report that the Division of Chemical Nomenclature and Structure Representation is supporting numerous projects and activities in our area of responsibility – Chemical Nomenclature, one of the core IUPAC activities, and probably the one which is most frequently associated with IUPAC.

Key project work includes further development of the IUPAC International Chemical Identifier (InChI) and Preferred IUPAC Names (PINs).

In the course of the development of the InChI one project has been funded so far this year: "Identifying International Chemical Identifier (InChI) Enhancements – QR codes and Industry Applications". A meeting on this project aiming at evaluating the needs of the users will also take place during the course of the ACS meeting in Boston. The Sub-Committee on the IUPAC International Chemical Identifier is the body through which IUPAC maintains oversight of the scientific activities of the InChI Trust. The chair of the InChI Subcommittee, Dr. Stephen Heller, has been awarded the ACS Patterson-Crane Award this year, indicating the importance of the work on the InChIs.

The Division has also been developing closer contacts with organisations which are or will be users of chemical nomenclature. Links with the International Organisation for Standardisation (ISO) resulted in a new project on developing nomenclature for carbon nanotubes and related nanomaterials. The ISO Technical Committee (TC 229) working in this area has been conducting a selection process for experts to participate in IUPAC projects, together with nomenclaturists from Division VIII. And a joint scoping meeting earlier this year made it clear that also a collaboration on nomenclature for metal clusters is highly desirable.

We also anticipate significant progress being made on developing Preferred Names for inorganic compounds and for polymers. The document "Specifying the Coordination of Ligands to Central Atoms: Detailed Description of Grammar in the Kappa (κ) Convention" shall be a first step in this direction. Also the document "Preferred names of constitutional units for use in structure-based names of polymers" will be submitted for review before the end of this year.

Other projects nearing completion are the "Nomenclature of Flavonoids" which will be resubmitted for publication soon, and the "Source-Based Nomenclature for Single-Strand Homopolymers and Copolymers" which was recently submitted for review. A main feature of this latter document is that only a limited

number of frequently encountered polymer names have been included as “retained polymer names”. Otherwise names of polymers shall be based on acceptable names for the monomers (or, in the case of structure-based names, on the accepted names for the constitutional units).

The revision of the nomenclature of carbohydrates is an ongoing project. Unfortunately during the course of the project we recognised that there are inconsistencies between the existing document and other documents, such as fullerene nomenclature or natural product nomenclature, regarding treatment of additional rings. This and the very sad passing away of a very competent task group member, Prof. Derek Horton, earlier this year has made it necessary to extend this project. The application is in preparation.

Since the IUPAC compendia on nomenclature are very long documents, such as the recently published new Blue Book, *Nomenclature of Organic Chemistry, IUPAC Recommendations and Preferred Names 2013*, with its over 1600 pages, we initiated projects on the preparation of Brief Guides which shall be handy leaflets, easy to include in author guidelines or to be reproduced in text books. After the 2-page Brief Guide to Polymer Nomenclature in 2012 we could just finalise the Brief Guide to the Nomenclature of Inorganic Chemistry comprising 4 pages. We look forward to completing the Brief Guide to the Nomenclature of Organic Chemistry (also 4 pages) in the near future.

Project Reviews and New Funding Committed

New projects approved so far this year are:

- Nomenclature for polymeric carriers bearing chemical entities with specific activities and names

- Nomenclature of Homodetic Cyclic Peptides Produced from Ribosomal Precursors

- Identifying International Chemical Identifier (InChI) Enhancements – QR codes and Industry Applications

Several other project proposals are in preparation, at least one of them concerning the preparation of a corrected or revised version of the new Blue Book.

Recent Publications Related to IUPAC Division VIII

R. G. Jones, T. Kitayama, E. S. Wilks, R. B. Fox, A. Fradet, K.-H. Hellwich, M. Hess, P. Hodge, K. Horie, J. Kahovec, P. Kratochvíl, P. Kubisa, E. Maréchal, W. Mormann, C. K. Ober, R. F. T. Stepto, M. Vert, J. Vohlídal, Nomenclature and graphic representations for chemically modified polymers (IUPAC Recommendations 2014), *Pure Appl. Chem*. **87**(3), 307 – 319 (2015); Erratum: *Pure Appl. Chem*. **87**(4), 441 (2015)

R. M. Hartshorn, K.-H. Hellwich, A. Yerin, T. Damhus, A. T. Hutton, Brief Guide to the Nomenclature of Inorganic Chemistry *Pure Appl. Chem*. **87**(8), xxx – yyy (2015); DOI: 10.1515/pac-2014-0718 (currently available online as ASAP publication).

Karl-Heinz Hellwich

President

IUPAC Division of Chemical Nomenclature and Structure Representation