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

Approved minutes of the Division Committee Meeting
Cambridge, UK, 4–5 August, 2016

1 Welcome, introductory remarks and housekeeping announcements

Karl-Heinz Hellwich (KHH) welcomed everybody to the meeting, extending a special welcome to those who were attending the Division Committee (DC) meeting for the first time. He also thanked the Royal Society of Chemistry for hosting the DC meeting and providing the necessary facilities. He described house rules and arrangements during the meeting.

2 Attendance and apologies

Present: Karl-Heinz Hellwich (President, KHH), Risto S. Laitinen (Secretary, RSL), Osman Achmatowicz (OA), Michael A. Beckett (MAB), Ture Damhus (TD), Phil Hodge (PH), Alan T. Hutton (Vice President, ATH), Robin Macaluso (RM), Gerry P. Moss (GPM), Warren H. Powell (WHP), Michelle M. Rogers (MMR), Molly A. Strausbaugh (MAS), Keith Taylor (KTT), Andrey Yerin (AY).

Observers: Jan Reedijk (day 2; JR), CCDC representatives (day 1; Clare Tovee, Stephen Holgate)

Apologies: Fabio Aricò, Ivan Dukov, Gernot Eller, Richard M. Hartshorn (RMH), Todd Lowary, Elisabeth Mansfield (EM), Leah McEwen (LRM), József Nagy, Ebbe Nordlander (EN), Jan van Lune, Jiří Vohlídal (JV).

No replies: Hyo Won Lee, Martin Putala, Amélia Pilar Rauter (APR).

3 Introduction of attendees

A short round of introductions was made. Robin Macaluso (University of Texas at Arlington), Molly A. Strausbaugh (Chemical Abstracts Service), and Osman Achmatowicz attended the meeting of the Division Committee for the first time.

4 Approval of agenda

Agenda was approved (Appendix 1) as modified.

5 Approval of minutes of meeting in Busan, Korea, 8–9 August 2015

KHH suggested several amendments to the draft minutes. In addition to noting several typographical errors and other technical corrections, he proposed modifications in the text. WHP suggested that the changes in the context should be enumerated in the minutes. The most significant changes noted by KHH were as follows:

- Item 8.1: RMH was asked to become a task group chairman not a subcommittee chairman.
- In the 2nd paragraph of Item 8.1, the mention of the three planned workshops was removed and the description of a new project proposal on InChI for mixtures by LRM was elaborated.
- The text in Item 8.3 and Secretary's comment under Item 8.7 were clarified.
- There were a number of errors in the Polymer projects (Item 8.16), namely in Items 8.16.1, 8.16.4, and 8.16.6, which needed to be corrected. There was significant rewording in each case.
- The text in Item 11.3 was clarified.
- Appendix 5: The proposal of the interchange of the list of members and their expertise in Divisions IV and VIII was added in the minutes (point 3). The discussion about a concurrent meeting was minuted as a point 4.
- Appendix 11: A list of proposed membership of Division VIII for 2016-2017 at the time of Busan meeting was added.

The minutes were approved as amended.

6 Matters arising

KHH suggested based on discussions between him an TD that specific actions that will be decided by the Division Committee should from this meeting on be separately minuted in each Item as appropriate. The action summary should also include information about who is to carry out the planned action.

KHH noted that in Busan it was agreed with Div. IV that we would exchange the list of members with keywords for their expertise. So far neither Division has produced such a list.

Suitability and acceptance of PINs will be discussed in conjunction with kappa terms under Item 8.8

> ***Actions:*** Div. VIII will prepare a list of our Division Committee membership together with a few keywords to define expertise, which will then be distributed to Div. IV. RM noted that the best place to inform the expertise of each member would be the internal directory of IUPAC. She proposed that the IUPAC Secretariat should be suggested to add a tab of expertise in the internal directory. A country code should also be added to telephone numbers. Each member of the DC is to send their information to the Secretary, who will then prepare the list.

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

7.1 IUPAC bodies

It was decided in Bangor in 2014 that there should be contact persons for interdivisional information exchange. Thus far no interchange of information has taken place between the Divisions, but the current contact persons 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).

Division III. The assigned contact person is Amélia Pilar Rauter. There is no report of Division III counterpart.

Division IV. Phil Hodge is the assigned contact person. Both PH and KHH are members of SPT providing natural overlap.

> ***Actions:*** Contact relationships need to be renewed. RSL will send messages to the Secretaries of the above-mentioned Divisions.

7.2 Other bodies

RSC: ATH, KHH, Jeff Leigh, RSL met with Stuart Goven, who is an IUPAC liaison person in RSC. The topic of discussion was cooperation beyond publication, in particular the joint organization of workshops and problems with communication between IUPAC and NAOs. Stuart Goven welcomed Division VIII to have meetings in Thomas Graham House also in the future.

European Patent Office: KHH described the brief meeting in Busan with a representative of the European Patent Office. While there was interest in cooperation in the form of workshops and there was some exchange of emails, no further follow-up has taken place.

> ***Action:*** KHH will refresh the contact and explore the possibilities for collaboration.

ISO: KHH reported that neither he nor RMH have had any contact with ISO after the scoping meeting that was held in London in January 2015. One project on carbon nanotubes (2013-056-1-800) is in progress. The task group has met twice (see Item 8.18). There is also a project proposal on nanomaterials prepared by Yasir Sultan of ISO (see Item 9.1).

CCDC. ATH reported that members of the Division Committee (KHH, ATH, TD, Jeff Leigh, RSL, AY) met with the representatives of CCDC in the premises of CCDC. The objective of the visit was to exchange information about the modes of operations of both Div. VIII and CCDC and to scope the possibilities for future cooperation in the development of a unified system of nomenclature. CCDC uses IUPAC nomenclature and it is the duty of Div. VIII to provide the tools to the work.

> ***Action:*** KHH will contact Ian Bruno of CCDC to explore the possibilities to use the CSD data for future developments of nomenclature of new classes of compounds.

CPCDS (Committee on Printed and Cheminformatics Data Standards): CPCDS is a standing committee of IUPAC. They are involved in the new website of IUPAC and InChI. In a recent meeting CPCDS expressed interest in closer contacts with Div. VIII. Of particular relevance is the project of InChI of mixtures (CPCDS wanted to review it). The contacts with InChI subcommittee needs to be intensified. The chairmen expressed the desirability for mutual interaction – for example cross memberships. In a recent meeting in conjunction of the annual meeting of CPCDS, Div. VIII was not invited or informed even though the meeting was concerned with structure representation.

TD: what is the role of CPCDS. KHH: they are responsible for cooperation with de Gruyter. They are responsible for standards for representation of electronic data in particular structural representations. AY: There is overlap with responsibility between Div. VIII and CPCDS. The problem is that programmers are not familiar with the representations we want to see.

> ***Action:*** KHH will explore further developments of cooperation and cross membership with the chairman of CPCDS

RDA Workshop March 1, 2016: AY reported on a workshop of RDA (Research Data Alliance)/CPCDS. RDA has members from 110 countries. One interest group deals with Chemistry research data. The objective of the meeting: (1) Chemical structures, how to standardize and check chemical structures in electronic format. (2) antology of chemical data, classification of terminology. There are two publications treating published structures, rules to make structural formulae unambiguous, etc. There were 30 participants. The meeting was hosted by EPA (Environmental Protection Agency). CPCDS is organizing a Subcommittee on Cheminformatics. They want to involve Div. VIII. Four projects. The drawn chemical structure should be searchable. ACDLabs has preliminary software for the purpose.

ICTNS: GPM is a titular member and TD is the representative of Div. VIII on ICTNS. TD reported that he has had no contact from ICTNS and has seen no documents. GPM noted that as a titular member he sees most documents, but he is not sure what the relationship between the Division representative and ICTNS should be. TD has not even seen a list of documents which have gone to public review.
KHH asked specifically for the chapters of a book on Green Chemistry, which he had been assured during the Bureau meeting in April, that he and TD would receive for checking. But TD has not yet seen them, whereupon PH stated that as a contributor to the book he had seen the page proofs.

Interaction with ICTNS must be intensified. KHH has been in contact with Ron Weir to discuss problems in interaction and communication. KHH has requested that in case ICTNS receives a manuscript that includes nomenclature, the Div. VIII representative should also receive the manuscript for review. KHH has been assured that it will happen, but apparently this has not been the case.

Many of the documents are sent to public review within two weeks after the document has come to ICTNS. Public review lasts five months, but ICTNS review through Manuscript Central lasts only four weeks. Therefore, acceptance from PAC could come long before public review is over, which cannot be allowed to happen. The Secretary General of IUPAC should be contacted to discuss this situation.

MMR noted that ICTNS should have better communication system about the documents in public review. Now information of documents under review comes almost at the end of the review period. KHH said that normally documents in public review should be notified in Chemistry International at the beginning of the period. Unfortunately the information is often published only two weeks before the deadline. Possibly the public review should also be announced in PAC. Also NAOs should get notifications. The problem is that the email list is not up-to-date. MMR and MAS noted that the NAO of the USA is the National Academy of Sciences but it will often delegate these matters to ACS. NAOs should get direct information, but it is unfortunately not forwarded to the ACS Nomenclature Committee.

KHH noted that the IUPAC website should have an automatic system to alert the community that a new document is under public review. The documents should also be publicly available. Fabienne Meyers is responsible for public review and will initiate the review. MMR remarked that the users should not be expected to look for the documents in several different pages. Further clarification is needed.

It was thought feasible that NAOs could set up mailing lists to whom the alert should be sent. There are also other problems with the IUPAC website, which are concerned with the sign-in procedure.

> ***Actions:*** Several different parties should be contacted: KHH and GPM will communicate with RMH, Ron Weir and Fabianne Meyers to improve the situation and TD will voice his dissatisfaction directly to ICTNS. MMR and MAS will also take the matter up with the ACS Nomenclature Committee.

JCBN: GPM is the chair and KHH, TD, and APR are associate members. There are several joint projects with JCBN. The enzyme sub-committee of NC-IUBMB that meets jointly with JCBN reported that in 2015 they had created 199 new enzyme entries, 61 entries were modified, 27 were transferred to another EC number, and 7 were deleted.

8 Updates on Division VIII projects

8.1 IUPAC International Chemical Identifier (InChI) projects

A report by Steve Heller together with the list of current projects is presented in Appendix 2. KHH reported a newly approved project by Leah McEwen. LRM had considered that due to a short time from the previous task group meeting the meeting in Cambridge was not necessary.

KHH noted that several InChI projects are formally completed. However, there have never been reports in PAC or elsewhere about the outcome of the projects. KTT remarked that the manuscript is still not ready for publication in PAC. AY reported that InChI for polymer structures is in process. The code still needs to be implemented with suitable software for imaging of the structures. The ChemDraw users and other people have been consulted. There is no established way to announce the results. Possibly a short announcment in Chemistry International.

> ***Actions:*** Further information should be obtained by KHH from Steve Heller and Alan McNaught. It could possibly be done as an article in CI.

8.2 Preferred names in the nomenclature of organic compounds (the Blue Book) (2015-052-1-800)

KHH: The task group met in Cambridge for two and a half days. The Blue Book 2013 was the final result in the project "Preferred names", which was officially started in 1993. It was soon recognized that a complete revision is needed and it was not possible to aim merely at preferred names. Consequently, the 2013 version was a completely new book. WHP/HF and later WHP alone carried out the final editing of the new version. Because of the time pressure from different instances, the editor had not sufficient resources to create a subject index. It was provided by the publisher, but it unfortunately contained a large number of unsuitable enties.

Since the publication of the BB2013, numerous errors and inconsistences have been reported. The errata list has been compiled by GPM in the URL http://www.chem.qmul.ac.uk/iupac/bibliog/BBerrors.html with an additional page for trivial textual and typographical errors. An extended list of contents has also been prepared and is available on this webpage. The correcting of the errors has taken two and a half years, and only about 1/3 of the errors have been dealt with yet. Often correction necessitates a complete change in the example or text.

There were also other kinds of inconsistencies for which simple errata listing was not sufficient and which necessitated a new project. This task group aims towards new supplements beyond errata. This also included an extended list of contents and a corrected index. The new edition should also be in a searchable pdf format. The objective is to get it out by 2019, but that is probably not realistic.

WHP: The idea behind supplements is to provide principles of given topics in one place. Supplement 1 is concerned with priming. He also proposed a new general rule for the index: nothing comes before something. That principle was approved by a unanimous vote.

Supplement 2 corrects the errors on ordering based on locants and priority. It needs only a rewritten introduction, formatting, and final editing.

Supplement 3 is under preparation and deals with stereochemical description and inconsistencies therein. The publication might not need full public review.

KHH: There was discussion with Janet Freshwater of RSC Publishing. They are not keen on a new edition and not interested in a revised version. The agreement was that when all errors have been processed, a pdf of errata will be published, which will be publicly both on IUPAC and RSC web pages. The next edition will be a two- or three-volume book with the index being the third volume. It is currently an option, but no firm decision has been made. The publication needs to be discussed between marketing in RSC and the treasurer and Secretary General of IUPAC.

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

GPM: Nothing new to report

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

GPM reported that the project is to name homodetic cyclic peptides produced from ribosomal precursors. A preliminary report has been prepared which is to highlight a proposal that the order in which the amino acids of such a peptide should be quoted is selected using the CIP rules. This is in contrast to existing systems that use alphabetical order. Thus proline is preferred to selenocysteine, to cysteine, to threonine, etc. The classification scheme that is presented shows that it includes many post-translation changes including depsipeptides and peptides where additional cyclisation has occurred. How these will be named has not yet been addressed. This project deals with a subset of compounds covered by Item 8.3.

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

GMP: No progress. The project has been passed to Kristian Axelsen. The different documents need to be connected. KHH noted that this is a long project (2006). There is a document that needs revision in the light of new BB and this will be a new task. GPM remarked that one reason for the revision is the bad organization of the initial document. There is a real need for a proper nucleic acid document, as the naming of nucleotides has become complicated. One important challenge is the naming of the morpholino nucleotides (i.e. synthetic polynucleotides). The new BB can point the way forward.

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

AY: The project was initiated four years ago as a technical report to compare different usage of hydro prefixes (CA, Beilstein, etc.). The document will be ready for review possibly in the beginning of the next year. The project will probably be finished by the end of next year.

8.7 Revision and extension of IUPAC recommendations on carbohydrate nomenclature (2012-039-2-800/2015-035-2-800)

GPM reported that the task group met in May. The continuing work concerns with di- and oligosaccharides and the goal is to connect the carbohydrate document with the glycolipid document. The symbolic code for carbohydrates is new and challenging. The two different systems, which have been used in the past, have now been unified. KHH: A lot of revision has been made but a lot of work needs to be done. APR is a secretary of the group, but it is not clear who should do the next version (GPM has prepared the previous version). A key task group member, Derek Horton, passed recently away but a new member, David Baker, has continued the work.

Action: KHH will produce a section on fused systems.

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

TD described the project, which was initiated a decade ago with the intention to get rapidly started with the discussion of inorganic PINs, at least for inorganic compounds that have ”drawn molecular structures”. It was realised, however, that the two methods designating ligating atoms in the ligands (the kappa and eta conventions) need to be developed further. A general procedure for selecting and ordering central atoms has also a higher priority.

Consequently there are two documents in preparation, the kappa document (which also discusses eta) and the central atoms document.

The kappa document was developed in a number of steps with RMH as the main author. At the appearance of each draft, problems were still identified, and the application of more and more complex kappa notations were suggested. The worst problem was generated upon applying multiplicative names for ligands as, *e.g.*, of the edta type. In the spring of 2016, it was agreed that TD would take over the role as the main author of the kappa document, freeing RMH for his new duties as Secretary General.

A brief draft document was hastily prepared by TD for the Cambridge meeting in August 2016. It contains new rules for the kappa convention and completely abandons multiplicative names for ligands. It is also suggested that kappa terms should be placed as close as possible to the part of the name specifying the ligating atom rather than collecting all kappa terms together after the complete name of the ligand. This approach removes the problem of finding locants that unambiguously specify the ligating atoms.

The new rules renders the kappa terms simpler to write and to interpret. All examples in the current document could be easily named using the new rules and fully substitutive names for the ligands (which were earlier named using multiplicative nomenclature). Repetition of name parts with different kappa terms makes for longer names, and PINs for organic ligands will in many cases not be the names used for the same compounds when they are ligands.

By way of example, ligand names for edta (the tetraanion) are always based on the fully substitutive name

***N*-{2-[bis(carboxylatomethyl)amino]ethyl}-*N*-(carboxylatomethyl)glycinate**

Examples where kappa terms are introduced:

N*-{2-[bis(carboxylatomethyl)amino]ethyl}-*N*-(carboxylatomethyl)glycinato-κ*N*,κ*O

N*-{2-[bis(carboxylato-κ*O*-methyl)amino-κ*N*]ethyl}-*N*-(carboxylato-κ*O*-methyl)= glycinato-κ*N*,κ*O

If the two carboxylatomethyl groups cited first in the name are coordinated differently, separate name parts are needed for them, as shown here:

N*-{2-[(carboxylatomethyl)(carboxylato-κ*O*-methyl)amino-κ*N*]ethyl}-*N*-(carboxylatomethyl)glycinato-κ*N*,κ*O

The new rules and names should be incorporated in the existing document, the drawn structures of which can still be used (but a few new ones need to be added).
Much of the existing text can also still be used.

Central atoms document: a commented incomplete draft exists. Due to the involvement with the kappa document there is no progress to report since last year. There will be a need for a new project on central atom selection. This will become relevant only after the kappa document has been

finished.

Inorganic PINs are far out in the future.

JR: How does this affect the Brief Guide? TD: The new rules will lead to revision of the Brief Guide.

> ***Actions:*** TD will incorporate the new kappa-principle into the existing document, which can be produced relatively quickly. After that a new project proposal on central atoms will be made**.**

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

ATH reported that the Inorganic Brief Guide was published in November 2015 and the four-page version has appeared in Chemistry International. There is a handout for the use by school teachers and students and for inclusion in chemistry text books. It can be downloaded from the project page in the IUPAC web page and reproduced provided it is done in its entirety. Several translations are also completed and accessible via the project web page on the IUPAC web site.

ATH reported that the Organic Brief Guide has taken longer to produce. The objective is to get it for review by the end of the year.

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

MAB reported that the task group has not met face to face, but there has been a lot of email correspondence and significant progress has been made. It was decided in March to submit the document for internal review. There are still some comments to be received. After that the revised manuscript can be submitted to PAC and external review.

TD pointed out that there is potentially a new need to mix additive and substitutive nomenclature in naming the metallacycles (see Item 8.11), and the changes in the use of kappa might impact on the borane document. WHP remarked that the publication of the document should not be postponed any longer, since it has already been a very long project.

KHH noted on the formality that all Division VIII documents should have a symbol followed by a hyphen. The borane document could thus be BN-*xxx*.

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

ATH reported that a partial metallacycle task group met in Busan in 2015 and produced a document, which formed the basis for the discussion in the task group meeting in Cambridge. If all changes that were suggested could be made, the document can be submitted for review by the end of 2016. The full task group met in Cambridge with the exception of Dan Rabinovich. The task group was complemented by Ed Constable, Jeff Leigh and TD.

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

KHH: The document was sent to ICTNS and public review two years ago. There were plenty of comments and significant extension of the document was requested (list of flavonoids and their InChI codes). The structures needed to be redrawn. KHH observed inconsistencies in examples and the task group needed to be contacted, since these inconsistencies need to be corrected. The document will be resubmitted to PAC after final editing by KHH in the autumn.

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

JR: The project is active and going smoothly and on schedule, but there has been no formal report. The document might be ready by Sao Paulo meeting.

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

TD: task group meeting will take place on Monday 8.8.2016 together with Dick Jones. It is a project that contains both terminology and nomenclature.

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

KHH: The project was dormant for several years. The original objective was to provide nomenclature rules for molecules of biological interest that are not covered in other documents due to the lack of suitable compound classes. GPM: The task group has been taken over by Marcus Ennis, but nothing much has happened.

8.16 Polymer projects (with Division IV)

KHH reported that the polymer Division had a meeting in July in Istanbul (SPT met in advance on July 12-15, 2016). There is no information on the outcome of the meeting.

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

The document was ready for review already last year. Internal revision was made and minor changes were suggested. The document was sent to ICTNS and public review during the Busan meeting. Comments by SPT and task group members necessitated two new revisions. Final editing was made by KHH and Dick Jones. A second round of reviews produced a request for major revision, but in fact the changes were only minor items. The accepted version still contains errors. They have already been corrected but the document needs to be checked carefully in the proofs stage.

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

PH reported signifigant progress and the document should have been sent to public review a month ago, but it is not clear whether the document has in fact been submitted for public review. KHH remarked that internal review had produced a number of comments. It was decided to restrict the discussion to simple cases, because irregular dendrimers will become very complicated and would be better dealt with in a follow-up document.

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

KHH: After the internal review and discussions in Busan the document has seen two revisions. It contains the same table in the appendix as the document concerned with source-based names. The document was extended (text, examples, explanations). The document has been sent to ICTNS and public review in April/May, 2016. The deadline of the public review is at the end of the year. There is a conflict between the length of the refereeing in PAC and public review. The paper was accepted for publication in PAC long before the public review was over. It was felt that this procedure obviously does not work properly. Hopefully the final version will be submitted for publication by the end of the year.

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

PH reported that the content material in this project keeps shifting and consequently little progress has been made. However, he was optimistic that the project should now be going forward relatively soon. KHH noted that there were no structures for many of the names in the Table, but he reported having added them from the draft document under Item 8.16.3. Upon redrawing of the structures unfortunate errors were introduced. After final editing, only formalities need to be completed. Since the document is planned to be only a web version, it might not need the PAC refereeing procedure.

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

KHH: Two years ago it was decided to make an addendum to the existing document, which contains errors. Since the Istanbul meeting, there have been two versions, which need to be reviewed by the task group, but the document can be sent to internal review by the end of the year.

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

KHH: The task group met in Istanbul, but there is no new draft.

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

GPM reported that there was a task group meeting in Istanbul, but no informtion of the progress prior to the meeting. However, the document needed a lot of work. The problem is that whereas components can be named individually, when they are combined, the naming becomes difficult. AY: The system is quite correct but still needs a lot of refinement. It is necessary to specify the site, where the molecule is linked to another molecule. GPM: The name of the project is currently “The Nomenclature and terminology of conjugates”. There is currently draft 6, but no information about the outcome in Istanbul. An observer, Paola Carbone, was recruited to the task group

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

KHH: No news since last year.

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

KHH reported that this project has only Email-meetings with Albert J. Dijkstra (AJD) as the task group leader. The document was submitted for review in April. The document was loaded to ManuscriptCentral before it was ready for review (it was not the latest version). Even though the submission should have been withdrawn, it has not happened. There are still plenty of errors and omissions in the revised document. The revision of the document is necessary because of the inconsistent use of the end-of-the-line hyphenation in the literature.

JR has contacted AJD by email and has received the response that the revision is proceeding and will be completed shortly.

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

KHH: The task group had a meeting in Busan and another one in February this year. AY reported that the meetings were fruitful, but there have been no reports. It has been decided to classify carbon nanotubes according to their sizes and number of walls. There is a need to be able to describe stereochemistry and isomerism, functionalization, etc. The document will be a short set of instructions, how to assemble carbon nanotubes. There is no draft as yet, only ideas and general outline. KHH noted that people with different areas of expertise (carbon nanotubes, nomenclature, polymer, etc.) did constructively work together towards a common goal.

8.19 Survey of Definitions and Use of common Solid-State Chemistry Terminology (2015-053-1-200)

RM reported that the group met online in March. This is mainly a terminology project. The aim is towards describing the bonding etc. with a strong educational aspect (see IUPAC webpage). There has not been a need for the task group to meet in Cambridge and everything was done by email and Skype. The next scheduled meeting is in January with the aim to have a document by that time. The third meeting will be a face-to-face meeting.

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

KHH: No news to report. GPM noted that this is not simply an exercise to transfer data from various documents to the Gold Book. Both editing and checking and correcting of the conflicting information is needed. There are ca. 100 publications with glossaries, which were prepared by different task groups at different times resulting in the formulation of the same information in different ways. The editing would be a huge task. TD suggested that each Division should have a glossary-representative in the similar fashion as the representative for ICTNS. GPM remarked that it is not clear how the Gold Book should be updated and who is in charge of it. KHH noted that the last printed Gold Book was published in 1997. Since then there have been attempts to produce the electronic version but it has not been continued. Somebody needs to become familiar with the existing material and be able to update the format and the content.
KHH reported that he had attended a Division VII meeting on November 9, 2015 in Tübingen, Germany, the topic of which was duplicate definitions (in the context of assembling a book out of

several single documents on terminology in the area of toxicology). The participants agreed that it is a huge problem and this task will need alignment beyond the boundaries of disciplines.

[Secretary's comment: No action was decided, however, on this item]

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

GPM reported that the project is concerned with the transition states in various transformations. There is a document by Michael Blackburn. The goal is to identify each phosphorus atom of the phosphate groups in enzymes and proteins. There is unfortunately no correlation in the names used upon different determinations of the crystal structures. The numbering of P-atoms should be standardized. One problem is that when oxygen is replaced by sulfur, chirality might be changed. The public review finished in June and the revised version is being produced. KHH noted that some recommendations from the RB have been ignored and need to be corrected.

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

KHH: A part of a large project, which was started decades ago. The first publication "Graphical representation of stereochemical configuration" appeared in 2006, and "Graphical representation standards for chemical structure diagrams" in 2008. The project has run out of budget. A new or extended project was drafted, but since there was no progress report, the project was rejected. KTT remarked that though the project run out of money and time, there is still a need to complete it. Therefore the project should be revived. KHH: In order to get an extension, a project report about the current state is needed. A new proposal can then be drafted. However, the number of task group members needs to be reduced and the project needs to become more focused. KHH noted that if there is a draft of a document, the progress report can be short.

Action: KTT to prepare the progress report and draft a proposal.

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

KHH: Nothing to report.

9 Future projects/activities

9.1 International Organisation for Standardisation (ISO) liaison. Nanoparticles projects (see also 8.18 above)

ATH reported that there was a scoping meeting with ISO in London in 2015. This resulted in two rough draft proposals: (1) Proposal by Yasir Sultan: Nomenclature of silver and gold nanoparticles, (2) Proposal by Edwin Constable: Nomenclature of large clusters. It is necessary to find right people, who have the expertise (people involved in InChI, ISO, this Division, ICTNS, Div. II, computational chemistry, Alison Smith, etc.). It was felt that the project on gold and silver nanoparticles is more suitable for Div. II (it needs to be discussed with Jan Reedijk). The problem is

that ISO has no resources for funding. EM is also involved in projects related to this item. KHH: Fullerene specialists need to be consulted in connection of the cluster project.

Actions: ATH will get back to ISO and ask Yasir Sultan to find suitable people.

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

ATH: The plan has been to produce a new RB by 2019, but it is an overoptimistic timescale. Up to present no definite project leader has been suggested, but there might be a need for the revised edition. There will be new documents, which need to be incorporated, and there will be new additions, modifications, and corrections. The solid-state chapter needs revision, and new information about boranes and metallacycles, the revision of the kappa convention, etc. need to be considered.

Actions: A project proposal possibly within 1-2 years.

9.3 Graphical representation of polymers

KHH: nothing to report

9.4 Rotaxane stereochemistry

AY: Nothing to report

9.5 Delocalised systems

TD and AY reported that this project has seen informal discussions and AY is ready to form a task group to consider tautomers and mesomers. TD is involved in the project because of the problem of assigning PINs to anions that are corresponding bases of several mutually tautomeric acids. However, there are rules in BB for the seniority of tautomers. Thus the senior tautomer is selected for naming the anion, which solves that particular problem.

9.6 Crown nomenclature

KHH: nothing to report; except that calixarenes should also be considered.

9.7 Central webpage for all IUPAC recommendations/publications

KHH: The new IUPAC webpage was lauched last April. There are still shortcomings, but now there are more sections on the front pages. Searches are still somewhat problematic. Brief Guides will direct to other documents. The home page should contain directly the title Nomenclature. The organization of the menu items also needs to be reconsidered. So in the near future it should be possible to envisage a structured access to all IUPAC rrecommendations.

9.8 Document on italic and roman fonts

KHH reported that this document was discussed in Busan. ICTNS was consulted, but errata was not published.

Action: KHH to contact ICTNS again for the publication of erratum or 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

There has been no progress on this project since Busan due to MMR's schedule. However, this is still an issue for industry and the project proposal needs to be completed before the 2017 GA in Brazil. In the subsequent discussion, it was indicated that this project ties to the work being done on the InChI of mixtures on one hand and to AY's potential project on variable substitution (see Item 9.10). MMR, AY, and TD expressed interest in the participation of the combined project for UVCB nomenclature and variable substitution.

Action: MMR will contact AY to initiate the discussion on a joint project.

9.10 Variable substitution

AY: There is need in industry, but IUPAC does not provide satisfactory rules. However, CAS has a system incorporated. KHH: Since there is a need, a task group could be formed.

Actions: Since four persons are interested (MMR, KTT, TD, AY), a task group could be formed

9.11 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: There is (seemingly) a plethora of different classes of names, but it is not clear what the difference is between the different classes. Only 2-4 classes are needed. This problem was discussed in Busan. KHH: It was considered in the BB task group what to do with widely used names that are not acceptable. For instance, phosphine for phosphane. It is important to be careful, how the displeasure against a certain name should be expressed. TD: The users expect clear rules, but then they might ignore them.

Actions: TD to prepare a working paper detailing suggestions for terminology.

9.12 Overall numbering of atoms of a compound

KHH: This is a general problem, which has been discussed in connection with carbohydrates, polypeptides, etc. GPM remarked that crystal structure determinations ignore IUPAC numbering.

Actions: AY will initiate a survey of the need for universal numbering in different fields of research.

9.13 Other projects

9.13.1 Project proposal on Ionic liquids (K. Seddon)

KHH reported that this project proposal was made in the early summer. There are already some comments. The project is mainly about terminology, though nomenclature is also mentioned. There is nothing new needed for nomenclature, but names in the document need to be corrected. This project cannot be a sole Div. VIII project. Div. II and III were asked to participate, but they declined and the project is now under review by Div VIII. RM noted that she can possibly get an expert in to participate in the project and expand the geographical distribution. JR observed that neither Div II nor III were enthusiastic, nor seems Div VIII to be. TD remarked that the review process should not involve bureaucratic formalities, only content. It is the task of the Secretariat to control the formalities. KHH noted that it is the members of the DC, who are responsible for the content of the project proposal and the project outcome. DC is mainly managing the projects.

> ***Actions:*** KHH will send comments to the Secretariat, and he encouraged every member of the DC to do so. The opinions can be sent either to KHH or Fabienne.

9.13.2

AY maintained that the decoding behind storing electronic information (chemical data standards etc.) is important. He maintained that it is not a project, rather an initiative.

10 Membership matters

10.1 Status of Division VIII Committee membership

KHH stated that the DC has three vacancies: One for AM and two for NR. MAS has been nominated as an AM to replace John Todd. She is currently an observer in this meeting.

> ***Action:*** The DC agreed unanimously to suggest Bureau to appoint MAS as AM.

KHH also noted that there are possibilities for an NR from Spain, but the process is still unfinished. EN Suggested a Brazilian, Ana Maria da Costa Ferreira, as an NR. KHH will contact her, and then the nomination from the Brazilian NAO will have to be obtained.

10.2 Division VIII representatives in other IUPAC bodies (CCE, PAC Board, ICTNS, COCI, JCBN)

CCE:	RM
PAC Board:	ATH
ICTNS:	TD
COCI:	MMR is the contact person
JCBN:	GPM (chair), KHH (ex officio), APR (AM), TD (AM)
CPCDS:	AY; KTT is a member

10.3 Division VIII Advisory Subcommittee

The Advisory Subcommittee was set up to include persons who could be contacted on specific questions of nomenclature. The webboard unfortunately does not work, and the list has not been updated. The updated contact details of the members, however, have been sent to the IUPAC Secretariat.

ATH suggested that known Advisory Subcommittee members should be contacted by email and asked whether they are willing to continue in the Advisory Subcommittee.

> ***Actions:*** RSL will undertake this task. How to activate and expand the Subcommittee? List of expertise should be collected. Minutes of the meetings should be distributed.

10.4 Nominating Committee

ATH agreed to be the chair. The composition of the Nominating Committee will be decided on later.

> ***Action:*** Those interested should show their interest with the understanding that they cannot become Titular Members if they participate in the Nominating Committee.

11 Status on Division VIII web board with discussion forums

The web board is not active. See also Item 10.3.

12 Publicity

12.1 Division VIII (and related) publications since the 2015 Division Committee meeting

The list of publications is shown in Appendix 3.

12.2 IUPAC-IUBMB nomenclature website

No report.

12.3 IUPAC website

The advantages and shortcomings of the new website were discussed throughout the meeting.

13 Reports from other IUPAC bodies

13.1 ICTNS

No report

13.2 JCBN

GPM: The progress was covered together with the projects.
There is a proposal to extend the tetrapyrrole document.

13.3 CCE

No report from the activities during the last year.

14 Any other business

14.1 Names of new elements

KHH: The document on the names for new elements is in the public review till November 8: 113 nihonium Nh, 115 moscovium Mc, 117 tennessine Ts, 118 oganesson Og. There is an objection to the element symbol Ts (conflict with the recommended abbreviation for tosyl), and the name tennessine is objected to by TD on linguistic grounds.

There was discussion with JR about the element symbol Ts and the name tennessine in general.

15 Dates and venue for next meeting

Division committee will probably meet on August 8-9, 2017 (or maybe August 7-8), during the General Assembly on August 6-13. The IUPAC Congress takes place on August 9-14. All these events take place in Sao Paulo, Brazil.

16 Adjournment

KHH thanked the participants and RSC and adjourned the meeting on 14.50.

Appendix 1

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

Draft agenda for Division Committee Meeting
Cambridge, UK, 4–5 August, 2016

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 Busan, Korea, 8–9 August 2015

6 Matters arising

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

8 Updates on Division VIII projects

8.1 IUPAC International Chemical Identifier (InChI) projects

8.2 Preferred names in the nomenclature of organic compounds (the Blue Book) (2015-052-1-800)

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

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

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

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

8.7 Revision and extension of IUPAC recommendations on carbohydrate nomenclature (2012-039-2-800/2015-035-2-800)

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

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

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

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

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

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

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

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

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

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

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

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

8.19 Survey of Definitions and Use of common Solid-State Chemistry Terminology (2015-053-1-200)

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

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

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

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

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

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

9.10 Variable substitution

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9.12 Overall numbering of atoms of a compound

9.13 Other projects

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10.1 Status of Division VIII Committee membership

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CCE, PAC Board, ICTNS, COCI, JCBN

10.3 Division VIII Advisory Subcommittee

10.4 Nominating Committee

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13.2 JCBN

13.3 CCE

14 Any other business

15 Dates and venue for next meeting

16 Adjournment

Appendix

Division VIII, membership roster for the biennium 2016–2017 (as of January 2016)

Name	Status	Term	NAO
Dr. Karl-Heinz Hellwich	President	2014-2017	Germany
Prof. Alan T. Hutton	Vice President	2016-2017	South Africa
Prof. Risto S. Laitinen	Secretary	2016-2019	Finland
Prof. Osman Achmatowicz	TM	2016-2017	Poland
Dr. Ture Damhus	TM	2016-2017	Denmark
Prof. Philip Hodge	TM	2016-2017	United Kingdom
Prof. Robin Macaluso	TM	2016-2017	USA
Prof. József Nagy	TM	2016-2017	Hungary
Dr. Michelle Monnens Rogers	TM	2016-2017	USA
Prof. Jiří Vohlídal	TM	2016-2017	Czech Republic
Dr. Michael A. Beckett	AM	2016-2017	United Kingdom
Prof. Ivan L. Dukov	AM	2016-2017	Bulgaria
Dr. Gernot A. Eller	AM	2016-2017	Austria
Dr. Elisabeth Mansfield	AM	2016-2017	USA
t. b. d. (nomination by CAS)	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	
Prof. Richard M. Hartshorn	*Ex Officio*	2016-2017	New Zealand
Dr. Gerard P. Moss	*Ex Officio*	2016-2017	United Kingdom
	10 TMs, 6 AMs, 8 NRs		

Appendix 2

InChI Trust Project Director's Report

August 2016

Summary:

Since the January 2016 report there continues to be good progress with InChI and the InChI Trust in a number of areas. Version 1.05 of the InChI algorithm was released for review in July/August 2016. Work on RInChI continues to move ahead. 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

Items covered in this report:

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

Membership/Support:

Summary

Two new organizations (University of California and Bio-Rad) have joined the Trust as Associate in 2016. Bio-Rad has been admitted in return for developing multithreading capability for the InChI software. IBM and PE have not paid their dues and have been removed. Discussions with EPA to join are proceeding.

As mentioned numerous times in the past in most organizations, since InChI works and it is not high on their immediate priority lists, actual real progress is slow without a dedicated champion within an organization.

As of August 1, 2016

Existing Members and Associates: 16

Supporters: 47

InChI RFP/Contracts

As has been the case for a long time, the contract for Markush structures with Digital Chemistry remains on hold awaiting potential funding.

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

InChI development work

Igor Pletnev continues to do a superb and a very responsive job as the InChI programmer.

IUPAC InChI subcommittee & working groups

IUPAC Committees

Chemical mixture composition

Leah McEwen at Cornell University 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.

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

Positional Isomers

Considerable technical interest in positional isomers has developed in the past 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 still 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. He has a put together a beta test version with some infrastructure and some test content .

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

Reactions –Under the programming direction of Gerd Blanke this project is moving ahead nicely.. There is an issue with how Google and other search engines index RInChIs.

Working group members are being asked to test the program with reactions from in-house databases or from RD files supplied on the web test site. After the successful conclusion of these tests and the incorporation of modifications, a beta test will be carried out by members of the SourceForge group. Thereafter, the first release of RInChI is projected to be in 2016.

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

Chairman: Gunther Grethe

Members:
Colin Batchelor
Jonathan Goodman
Hans Kraut
Martin Schmidt
Keith Taylor

Markush – With no interest from the US and other patent offices, this project remains on indefinite hold.

Electronic States – Don Burgess at NIST has developed plans for using InChI for Representations of Species at the Molecular Level. In 2014/2015 he 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. There still are no further developments here.

InChI for Materials – There is still no news from the NIST staff about this.

Organometallics- Colin Batchelor and his working group expect a final report in 2016. They are having discussions with the Inorganic working group as there is considerable overlap.

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

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

Nothing has happened since the October 2014 working group meeting at NIH as Keith Taylor was waiting for the extensions of InChI past 1024 atoms. With this now accomplished it is hoped progress will follow.

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

Chairman: Taylor, Keith

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

Tautomers. – Under the leadership of Marc Nicklaus, NIH/NCI, InChI project #2012-023-2-800, "Redesign of Handling of Tautomerism for InChI V2" is approved for funding by IUPAC. Marc plans to hold a working group meeting on this at the Philadelphia ACS meeting in August 2016.

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. Richard Hartshorn is leading this project. This is the announcement for this project:

"The InChI Trust (http://www.inchi-trust.org/) is examining development of a QR code (2D bar code) version of the InChI. We wish to consult with industry/regulatory/academic sector users to identify and 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."

January 2016 – June 2016 activities

Meetings Attended; Talks/Posters Presented

A number of conference call meetings with David Evans, Richard Kidd, and Alan McNaught were held over the past six months to deal with issues that needed to be addressed between Board meetings.

I met on a regular basis with members of NIH/NCBI, particularly Evan Bolton, to discuss InChI issues.

While in London for the Trust Board meeting I met with the staff of J. Cheminformatics regarding InChI publications. The InChI publications have very much helped their impact factor. I also met with Henry Rzepa. My EBI meeting was canceled at the last minute, but I continue to have productive interactions with EBI staff, notably Dominic Clark.

I attended the spring ACS meeting in San Diego and had a number of productive conversations and meetings.

In April I attended the BioIT meeting in Boston and presented a talk on InChI as part of a session on InChI for large molecules. Others speaking there were Keith Taylor, Evan Bolton, Larry Callahan (FDA), and Tyler Peryea (NIH).

In May I visited the offices of John Wiley in Hoboken, New Jersey and gave a lecture on InChI.

We hope to have another similar session at the 2017 BioIT meeting.

Manuscripts

There was an announcement about the InChI project in the June 2016 issue of the CDISC newsletter.

http://content.yudu.com/web/2htg1/0A2hthm/2016Q2/flash/resources/index.htm, Pages 4-5.

I would like to express my thanks to Dominic Clark at EBI for helping to arrange this note in the CDSIC newsletter.

InChI Trust web site

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

InChI Usage

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

InChI Trust Videos - Access numbers:

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

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

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

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

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

Representing Chemical Structures on computer – 675 (7/16); 546 (1/16); 390 views (7/15)
https://www.youtube.com/watch?v=uzXkJ9BsyHQ

(InChI part starts at about 14 ½ minutes into the video

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

Technical Issues

The mechanism to discuss and resolve technical issues continues to work well. 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 2016 and 2017

For the second half of 2016 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 Philadelphia. Give an invited talk at the Skolnik Symposium, and meet with groups to discuss adoption and usage of InChI.
4. Attend the November 6-8, 2016 Fulda meting and give either a poster talk or a lecture.
5. Attend the September 28-29, 2016 CDISC International Exchange meeting in Rockville Maryland (https://www.cdisc.org/interchange) compliments of CDISC which will cover the $990 registration fee.

2017

The InChI Standard has celebrated its tenth anniversary in 2015, and, building on the past and ongoing work by its working groups, a three-day meeting will be held next year on 16-18 August 2017 (Wednesday-Friday) at the main National Institutes of Health (NIH) campus in Bethesda, MD (short Metro/Subway ride from downtown Washington DC) The meeting will bring together the current InChI community and working groups that define the current state of the InChI project, together with other interested stakeholders. The aim is to discuss what is needed for the chemical, biomedical, materials, and related academic and industry communities for proper and useful structure standard representation of both small and large molecules, and the future direction and activities of InChI development will be a major goal of the meeting.

Steve Heller

Appendix 3

Publications since the last meeting in Busan (August 2015)

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P. J. Karol, R. C. Barber, B. M. Sherill, E. Verdaci, T. Yamazaki, Discovery of the element with atomic number Z = 118, completing the 7th row of the periodic table, *Pure Appl. Chem*. **88**(1 – 2), 155 – 160 (2016)

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L. Öhrström, N. E. Holden, The Three-Letter Symbol: Meddling Manner of Diplomatic Defusion?, *Chem. Int.* **38**(2), 4 – 8 (2016)

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H. S. Rzepa, A. Mclean, M. J. Harvey, InChI As a Research Data Management Tool, *Chem. Int.* **38**(3 – 4), 24 – 26 (2016)

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