

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

***Minutes of Division Committee Meeting
Bangor, UK, 3–4 August, 2014***

1. Welcome, introductory remarks and housekeeping announcements

KHH welcomed the attendees and thanked Mike Beckett for hosting the meeting at Bangor University.

2. Attendance and apologies

The following members of the Division Committee attended: Karl-Heinz Hellwich (president, KHH); Richard Hartshorn (past president, RMH); Ture Damhus (secretary, TD); Andrey Yerin (AY); Phil Hodge (PH); Risto Laitinen (RSL); John Todd (JT); Alan Hutton (ATH); Michael Beckett (MAB); Gerry Moss (GPM). Warren Powell (WHP) attended as an observer.
(On day 2, RSL and WHP had to leave early.)

Apologies had been received from:

Antony Williams (AW), Amélia Rauter (AR), Ebbe Nordlander (EN), Gernot Eller, Kirill Degtyarenko, Hinnerk Rey (HR), Md. Abdul Hashem, Michelle Rogers, Jiří Vohlídal, Lidija Varga-Defterdarović, Todd Lowary.

3. Introduction of attendees

A short round of introductions around the table was made.

4. Approval of agenda

KHH asked to add an item so that he and RMH could give the committee a 'state of the union' update. (This now appears as item 6a below.) Otherwise, the agenda was approved.

5. Approval of minutes of meeting in Istanbul, Turkey, 9–10 August 2013

The secretary had not been able to travel to Istanbul, and KHH thanked ATH for having agreed to write the minutes. The minutes had been circulated beforehand and there were comments from KHH and TD. The remark in item 6b about the Division's finances was to be changed so as to read that there had been a cut amounting to 15 % of 80 000 USD.
With the proviso that this be reworded and appropriate corrections of names and a few typos be made and some links and references be checked, the minutes were approved. TD was to finalise the minutes as described and place them on the Division web page with the assistance of the secretariat.

6. Matters arising

Regarding item 15.3.2 of the Istanbul minutes, RSL remarked that in the 80's when the periodic table with the 18-group format was developed by IUPAC, this happened on the request of the Bureau, so that at that time the table was, in fact, considered to be 'IUPAC business'.

[*Secretary's remark:* In the 1990 Red Book there is an Appendix commenting on various formats of the Periodic Table. The numbering of columns from 1 to 18 is labeled 'IUPAC 1988'. At the front of the book, an 18-column layout of the table is reproduced, entitled 'IUPAC PERIODIC TABLE OF THE ELEMENTS', a footnote assigning copyright to IUPAC and Kurt Samuelsson in 1985. The Appendix states that the Commission on Nomenclature of Inorganic

Chemistry had concluded that the 18-column format provided 'a clear and unambiguous labelling for reference' *within the Red Book* (my italicisation). The Appendix also explicitly encouraged members of the chemical community to voice their opinion on the periodic table (their 'local consensus' as it was worded) to the Commission.

The *Red Book 2005* reproduced the same format of the table and used the numbering of the 18 columns throughout the book without engaging in any discussion of various formats.]

AY suggested that Division Committee minutes in the future should be more informative regarding when and where task group meetings had been held. There could be a specific section of the minutes summarising such information which might be otherwise buried in reports or minutes from the individual task groups. The secretary said he would be happy to compile such a section but that it was up to the task groups to deliver the information, and this did not always happen.

6a. State of the union: report from the president and the past president

[This summary is based on the information given by RMH and KHH at the meeting and written notes given by KHH to the secretary immediately afterwards.]

The *proposed* (but at the time of the meeting not yet approved) schedule for the General Assembly (GA) in Busan in 2015 had an additional Bureau meeting included between Division Committee meetings and Council. Also the DC meetings were planned to start a day later. This meant that task group meetings and, not the least, the 3.5-day long meeting of the Subcommittee on Polymer Terminology (dealing with all the polymer nomenclature projects) would not be possible after the DC meeting. On the other hand, holding all these meetings before the DC meetings would cause additional problems concerning membership overlap of task groups and finding the necessary facilities (task groups would have to organise meeting rooms themselves).

Cross-fertilisation of Division Committee and projects might be reduced if task groups could not meet or decided not to meet at the GA because of these organisational problems, and maybe also because of financial restrictions.

KHH had been told by Fabienne Meyers that the changes had to be made for reasons of insufficient funding, but KHH said it must be cheaper to have the task groups meet at the GA's where a number of members were going anyway, and he feared that the proposal might lead to less participation in the GA.

RMH pointed out that it still is only a proposal. He also stated that working in task groups is an important route for new people to get into the IUPAC organisation.

RSL expressed concern that IUPAC is becoming a 'bureaucratic machine'.

RMH said IUPAC is struggling financially due to reduction in yields from investments and lost income from *Pure and Applied Chemistry*. Designing new subscription packages of IUPAC publications could perhaps increase interest among potential subscribers.

It was remarked that perhaps more use should be made of facilities at local universities when arranging IUPAC meetings.

KHH reported that after the resigning of René Deplanque as well as that of John Petersen, the union currently had no Secretary General and no Managing Director at the secretariat. Colin Humphris was acting Secretary General and also took care of some of the tasks at the secretariat together with Fabienne Meyers and the treasurer, John Corish.

PH asked how many staff should ideally be working at the secretariat and the reply was six.

While the Division Committee was contemplating this information, the message came that Dr. Lynn Soby had taken up the position as Managing Director.

Regarding the IUPAC web site, see item 13.3.

ATH remarked that the work we do is distributed via PAC and it must be accessible. GPM replied that even after the new agreement with de Gruyter, the technical reports and recommendations are freely available electronically. KHH and RMH will express to Bureau that we wish them to ensure continued availability of our recommendations.

ATH mentioned that the NAOs do not get sufficient information from the secretariat, and GPM agreed. KHH said it had been mentioned at the Bureau meeting in April that the NAOs would be informed about the changes in IUPAC management.

RMH further told that Bureau was working at a strategic plan. RMH will make a plea for nomenclature being part of IUPAC's future strategy.

RMH had submitted a proposal for a new election timeline for the Division Committees and Standing Committees. They should start later and be more focused. A nominating committee must be formed beginning of next year (2015).

[*Secretary's remark:* Shortly after the Bangor meeting, a message came out from Fabienne Meyers stating that there was general agreement that the timeline of the elections should be revised. A notice regarding the next election cycle had been posted on the IUPAC web site at <http://www.iupac.org/news/news-detail/article/iupac-elections-for-the-2016-2017-term.html> and an equivalent message was to appear in print in the *Chemistry International* September issue.]

Electronic voting mechanisms (*e.g.*, clickers) were being considered for the voting at council meetings.

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

Division II President Jan Reedijk had informed KHH that Daniel Rabinovich would be the liaison from Division II to Division VIII. It was decided that ATH should be his counterpart from Division VIII.

Daniel Rabinovich will be put on our mailing list.

A general discussion followed about contact persons for interdivisional information exchange.

A formal construction is not needed for colleagues from other divisions to participate in our meetings, since we always welcome observers.

It could be a task of the contact persons to go to the divisional cross-over-meetings at the general assemblies.

In terms of contact person from other Divisions, it was then decided to appoint Amélia Rauter as contact person for Division III (provided she agrees); PH agreed to be contact person for Division IV (it was remarked that both KHH and PH are in good contact with Division IV via their work in the Division IV Subcommittee on Polymer Terminology); and finally AY agreed to be contact person for Division I. Roberto Marquardt would be the counterpart to AY in Division I.

GPM remarked in passing that Division I is looking at semi-continuous updating of the Green Book.

8. Updates on Division VIII projects

8.1 IUPAC International Chemical Identifier (InChI) (2007-052-1-800) and related projects

[*Secretary's note:* the number 2007-052-1-800 is not in the project list on the IUPAC web site.]

Due to several cancellations, there had not been and would not be any InChI task group meetings in Bangor. No report had been received from the InChI subgroup.

[*Secretary's remark:* It turned out afterwards that the E-mail address of Steve Heller, chairman of the InChI Subcommittee, inadvertently had fallen off our Division E-mail list. The contact was reestablished, and Steve Heller soon after the Bangor meeting sent the 2014 InChI report which is included here as Appendix C.]

AY offered to report briefly.

He stated that by now virtually anyone working with the exchange of chemical information knows what an InChI is. Any software provider will enable use of InChIs to link to ChemSpider *etc.*

CAS also recognises InChIs. JT promised to go back and check details on CAS' support for InChIs.

[*Secretary's remark:* JT's findings arrived by E-mail a few day later and were as follows:

- In SciFinder you can import a structure from an InChI or a SMILES string in both the Java and non-Java structure editors.
- InChI strings cannot be searched using the Substance Identifier or Research Topic fields.

- Structures cannot be exported as InChIs, nor can InChIKeys be calculated for them.
- Neither STN nor new STN supports searching or exporting InChIs or InChIKeys.]

Current subjects worked at in the several InChI task groups included tautomerism and inorganic and organometallic structures. Only a year ago structures like ferrocene were incorporated and not much progress had been made lately.

There had been three meetings on InChIs for polymers; AY stated that rules for polymer nomenclature are "not so algorithmic". Nevertheless, the project had been completed.

Various IUPAC bodies present different wishes for InChIs.

Keith Taylor, working with biochemical applications, had contact to Pfizer and Roche regarding their systems for registering biological molecules using the SMILES-like so-called HELM notation (**H**ierarchical **E**ditin**L**anguage for **M**acromolecules), which is now public.

An InChI trust meeting was coming up in San Francisco (RMH to participate), followed by an InChI symposium at the ACS meeting.

AY gave a short report about recent extensions of the mol file format.

[*Secretary's remark:* A summary will be prepared by AY and added as an appendix to the minutes of next year's meeting.]

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

The Blue Book had appeared in print around New Year 2013–2014 and all joined in congratulating WHP for his accomplishments in completing this gigantic project.

WHP explained that the project was started around 1993 by Henri Favre; WHP had only joined the project in 1998. In 2003 a request was made for a separate chapter on the construction of preferred names.

The published book had turned out to contain a number of errors, many of these just minor ones (missing enclosing marks, excess spaces *etc.*), and WHP remarked that there had not been enough eyes on the final manuscript to help detect such typos and errors. The part on stereodescriptors had been the responsibility of Henri Favre and there had not been sufficient time to check it carefully. It would have been good to have had 6 months more to complete the entire task, but there had been pressure from the publishers and others to get the book published in 2013.

There were around 500 errors on the errata list by now. There was some discussion about the relevance of including the more trivial corrections. KHH said the errata list ought to be published on the web site for the Blue Book soon now. He hoped to have a final list by September to present as a PDF file.

The URL for the errata list is <http://www.chem.qmul.ac.uk/iupac/bibliog/BBerrors.html>

The index prepared by RSC was disappointingly bad both with respect to content and setup. Users would be better helped by using the table of contents.

ATH asked whether we should have a project to create a (publishable) index. Another proposal was to also prepare an "index guide" rather than just an index.

GPM said we should correct the errors we know of before publishing the PDF version of the book. There was a discussion about the publication of a PDF file based on WHP's corrected word file vs. the printed book.

GPM asked whether perhaps a project should be established to create the PDF file? We need to see what the contract with RSC says.

The book is advertised at £ 175 on the RSC homepage (<http://pubs.rsc.org/en/content/ebook/978-0-85404-182-4#!divbookcontent>), but it was remarked that it is also available more cheaply on the internet.

RSC does not seem to promote the book heavily. For example, it would have been good to have some flyers to distribute.

KHH was frustrated that the article about the Blue Book in *Chemistry International* (July 2014) had been editorially shortened and an error introduced in Henri Favre's name.

In the article it was published that we have set up the contact address bluebook@iupac.org.

Paul LeClair from the secretariat was only able to forward incoming mail from the community to *one* E-mail address, so KHH had created such an address in his own name and the messages will be further distributed from there to whoever is in the working group at any given time.

The procedure for replying to externals is a bit more tricky.

A detailed explanation about the use of bluebook@iupac.org had been sent to bluebook@iupac.org by KHH on July 25, 2014.

Two translations were being made; GPM was in contact with the Polish translator but would like to get in contact with the Japanese translators as well. Together with Fabienne Meyers, KHH had approved a Catalan translation of the Blue Guide (with the condition that the appearance of the new Blue Book be mentioned in the translation).

There had been a separate Blue Book meeting two days before the Division Committee meeting. GPM reported from that meeting that details had been discussed that may need attention when preparing the errata list and eventually the PDF file version of the book:

The handling of large numbers of primes will be added as a paragraph P-16.9.6 to explain the breaking into groups of three.

There is a problem in P-14.3.5 which needs further study on the order of letter locants which include superscript numbers and/or primes.

A footnote will be added to Table 2.5 (page 144) to explain for those entries with two suffixes when each of them is used. [It is explained in P-22.2.2.1.5.1 and P-22.2.2.1.5.2.]

An additional sentence will be added to P-25.4.2.3.2 to explain the direction of numbering.

Amine names, in particular P-62.2.2 on secondary and tertiary amines, had spurred quite some discussion. Having to use enclosing marks in a name like (triethyl)amine was considered unrealistic. KHH said if changes were made to this rule, however, we should check consequences for the rest of the book. It was not entirely clear what the next step would be regarding the amine names. It might be useful to set up a project to consider the problems. In this context, GPM would contact Ted Godly who had produced a document on amine nomenclature some years ago.

A technical problem arises if a corrected structure takes up more space than the previously printed one.

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

GPM had nothing to report. One section is missing and the document needs to be modernised.

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

At the JCBN meeting in May 2014 in Utrecht, it was decided to try to establish a project group. The document has been circulated to interested persons.

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 after the task group meeting on August 1 in Bangor, corrections and additions were to be made and comments taken into account, and after another round the document was expected to be in good shape. JT was to go back and have a CAS nomenclature expert validate the names in the draft.

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

KHH reported that the task group had met in Utrecht in May 2014. The project is about revision of the 1996 carbohydrate document, and Derek Horton had made progress on this. There was not much to correct; it was mainly about expanding the treatment of disaccharides and polysaccharides. There could also be issues about graphical representation of saccharides.

The needs of glycoinformaticists and carbohydrate synthesis chemists had to be considered and consistency with the phosphorus document (item 8.4) must be ensured.

GPM noted that there had been a discussion of the fundamental question 'what is a carbohydrate'?

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

The task group leader RMH noted that the project funds had been spent and the project was behind schedule.

The document on the extension of the kappa method for specifying ligand-to-central atom bonds needed minor repairs but was basically in place.

In this context, WHP mentioned a recommendation that he had made several times (beginning when Ted Godly was Secretary of CNIC). It involved the (not yet completely defined) principle that a coordination site takes precedence in a way similar to, but not exactly equivalent to, principal characteristic groups as used in organic nomenclature. All other neutral or ionic groups would be cited as substituents to the parent structure that contained the principal coordination site. WHP mentioned that he had applied this concept to all examples in last year's draft of the kappa document and that it did work. He felt that the kappa document was getting too complicated and that the suggested approach offered a simplification that should be fully explored.

Good progress had been made on the document on the selection of central atoms.

A task remained: to provide a list of retained non-systematic or not fully structural names that would be selected as PINs. At this point, TD remarked that he had considered this task again; it would be largely about compounds or entities for which only compositional (stoichiometric) information, or even incomplete such information, is available (or is conveyed by the traditional name) and that he was in doubt whether it would in fact be worthwhile to decide on PINs for such compounds. He argued that in many such cases the PINs were not likely to be used by the parties usually assumed to want PINs, *i.e.*, regulatory and customs authorities, patent lawyers, *etc.*

RMH and TD recalled an earlier discussion of the possibility of having PINs at various levels, for example, stoichiometric PINs, molecular PINs and structural PINs (other designations could be chosen) and TD asked whether there was a real need for PINs other than structural PINs which would be analogous to the organic PINs now given in the Blue Book.

RSL mentioned that the Commission on the Nomenclature of Inorganic Chemistry had resolved in the 90's that there was no need for inorganic PINs.

GPM noted that there is precedence for non-PIN areas in Chapter 10 of the Blue Book.

KHH suggested it might be better to establish some new projects with new titles. RMH stressed that in order to receive funding for such projects, the task group would have to produce something first.

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

An informal task group meeting had been held on August 2.

RMH reported that the inorganic document had been submitted and hopefully the restricted review needed for it (it involving no new recommendations) would be completed within a few weeks.

Members of Division II had also asked for, and had been given, copies for inspection (Javier García-Martínez and Jan Reedijk). KHH reminded that CCE should be given a chance to review the document.

Regarding the organic essentials document, although there was an advanced draft by now, it had been decided to attempt a quick rewrite of the beginning of the document.

KHH mentioned the possibilities of further brief guides on carbohydrate nomenclature, polymer terminology *etc.* – on the other hand we should not have hundreds of brief guides!

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

Some members of the task group had met in Bangor on August 1. MAB was happy about the progress made. There had been some discussion about terms like 'conjuncto' and 'supericosahedral'. The document that had been called 'the composite report' was being worked up to become a recommendation.

It was remarked that current debate over structural descriptors was based on electron counting rather than structure.

MAB would arrange a meeting in Prague later in August with members of the task group who could not come to Bangor; he would then present the project at the boron conference there and revise the document according to feedback received. The next task group meeting would then be at the 2015 IUPAC General Assembly.

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

It had been planned to have a meeting in Bangor, but the remaining budget had not allowed for this and the task group leader Bill Town had cancelled in the last moment.

The latest version of the document was version 5.1 from January 2014. There had been a meeting in Istanbul in 2013, and extensive E-mail work should have been done. RMH remarked that it was still 'work in progress', but that a new project application would have to be sent in in order to continue the work.

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

A scoping meeting had been held in Istanbul and a task group meeting the day before in Bangor. ATH noted that there were things to be done and the next meeting would be at the 2015 IUPAC General Assembly.

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

The document had been finished last year and submitted for review and had received many comments from the reviewers. A new draft had been discussed in Utrecht in May 2014, and a revised version had then been circulated in the task group with a request for comments before Bangor, but there had been no further reactions. The deadline by *Pure and Applied Chemistry* for resubmission of the revised manuscript had been exceeded.

AR was hoping for remaining comments to arrive at least by the end of August.

8.13 Coordination polymers and metal-organic frameworks: nomenclature guidelines (2009-012-2-200).

Document had been published [*Pure Appl. Chem.* **85**(8), 1715–1724 (2013)]. It is a terminology document.

There is a continuation in the new project 2014-001-2-200: Terminology guidelines and database issues for topology representations in coordination networks, metal-organic frameworks and other crystalline materials. This project is jointly funded by Divisions I, II and VIII.

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

There was basically nothing to report. The task group leader Dick Jones had been busy elsewhere and only some introductory terminology discussions had been held.

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

KHH reported from the JCBN meeting in Utrecht that there was basically no progress. The document is in database format and is not the right format for publication the usual way.

8.16 Polymer projects (with Division IV) [see also items 8.13 and 8.14 above].

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

KHH told that this was a very old project, but unacceptable names had kept turning up. Dick Jones had taken over after the chair did not turn up any more. Following advice and guidance received at the meeting of the task group last year in Istanbul, the 13th draft of the document was produced. This received further useful input from task group members and an extended critique from one in particular. Dick Jones prepared a response to the latter, which was circulated along with the 14th draft *medio* May 2014 with a request that task group members should consider any contentious issues and send comments and observations to Dick Jones within the same month. No such reactions were received and therefore he had advised the Chairman of SPT that the document was now ready for circulation to the full membership of SPT and the members of Division VIII. However, several comments coming late led to two further versions within the last two weeks, the latter of which still contains a considerable number of monomer names no longer retained in the Blue Book. TD agreed to assist KHH in the specific task of correcting the monomer names in the document within two weeks.

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

KHH detailed the recent history of the document which had been now submitted to ICTNS and was under review:

After the Istanbul meeting, the 13th draft was prepared. This was circulated for comments and observations from task group members, which in all but one case were received by the due date. Changes were incorporated, and the 14th draft was prepared. This was considered to be the final draft, so in concordance with agreed practice and support from the SPT Chair, it was circulated not only to task group members but also to the full memberships of SPT and Division VIII for their comments and observations. A number of responses were received and, where reasonable, every effort was then made to take the observations into account; of particular note were suggestions from JV, MV and JK from within SPT, and from AY and TD in Division VIII. At this stage, everyone with a right to comment had had ample opportunity to express their views, so the 15th and truly final draft was prepared. KHH had then had still some remarks about the structure of the document, some possible ambiguities and some residual nomenclature issues. After working in also advice given by other task group members, all outstanding issues were eventually reconciled in the 16th version which was submitted for ICTNS review.

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

Significant progress had not been made since last year. The task group had met in Istanbul without the chairman and had identified some problems. A new draft using a kind of substitutive nomenclature had been considered at the SPT meeting 4 weeks ago. The document may not be ready before end of next year.

Mistakes had been found in the document as well as complicated examples that were very difficult to name. The task group had decided to give dendrimers two names: one based on an old system where the names are simpler, and another one based on a new system, where the name is more complicated. The goal was now to complete a new draft by September.

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).

The project is on preferred names for constitutional units in structure-based polymer names. The document was to contain a table of retained polymer names. So far, a table had been created with acceptable names and unacceptable names. Additionally, a list of commonly used polymers had been created. Some names had to be clarified based on the new Blue Book about preferred names for monomers. The goal was to have the project finalized within about a year.

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)

PH currently had the final draft of this document from the task group. As required, it was now being more widely circulated for comments. PH was thus hopeful of having the final document very soon.

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

The document is half nomenclature, half definitions/notations/structure representation. It had not been progressed since Istanbul. KHH related the history of how he came to join the project. At the latest task group meeting, it had been concluded that the composition of the group and the workload did not allow for preparation of the document. The possibility to quit the project altogether or create a short addendum to the original document – instead of creating a new revised document – was discussed. It was decided that an addendum should be created. The task group members decided upon 5 topics that would be included in the addendum. The goal was to finish the draft addendum by the end of the year.

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

The document had been submitted for publication, unfortunately without waiting for comments from KHH. Also, it was a problem that corrections had not been carried over from version to version.

The published version is:

'Abbreviations of polymer names and guidelines for abbreviating polymer names (IUPAC Recommendations 2014)', J. He, J. Chen, K.-H. Hellwich, M. Hess, K. Horiea, R. G. Jones, J. Kahovec, T. Kitayama, P. Kratochvíl, S. V. Meille, I. Mita, C. dos Santos, M. Vert and J. Vohlídal, *Pure Appl. Chem.* **2014**, *86*(6), 1003–1015.

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

The task group chair had prepared a draft document for a task group meeting during the SPT meeting in Chiang Mai (Thailand) four weeks earlier. A long discussion had taken place on how a preferred CRU would have to be chosen. In order to come to a uniform solution, a joint meeting with the dendrimers task group (see item 8.16.3 above) had been arranged. The principle would be 'outward naming' of polymer chains (and dendrons) also when used as substituents.

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

There was already a draft document. There are two aspects: where is it desirable to split a given name, and how is this done technically. There was some discussion about the symbols to be used for line breakage. GPM mentioned the problem of breaking URL's.

As to the symbols to be used it was mentioned that the triangles used by Jeff Leigh in the Principles book were explicitly stated to be used in this book only. This sounded somehow different in the series of articles he wrote for Chemistry International. The Red Book 2005 used a set of horizontal opening and closing parentheses, *i.e.*, two horizontal curved lines. The German translation of the 1990 edition of the Red Book used an equals sign (=) for the same purpose, while the 1990 Red Book itself used a normal hyphen.

It was therefore concluded that a section on symbols used for these purposes would be helpful. But it should be made clear that in a normal printed document such as a research article in a journal the normal hyphen should be used when dividing a name. The other symbol(s) should be restricted in their usage for educational purposes.

The Division Committee agreed to the suggestion of WHP to divide names that contain locants always *in front* of (the) locants.

The project is run entirely via E-mail.

8.18 Nomenclature of carbon nanotubes and related substances (proposal 2013-056-1, Mansfield).

The project had been very recently approved (2013-056-1-800), but there had been no activity yet and an informal meeting on August 2 in Bangor among some of the Division Committee members had only dealt with some formalities. AY mentioned the membership. Three task group members come from ISO.

8.19 IUPAC Color Book Data Management (proposal 2013-052-1-024, Kinnan).

GPM had seen the list of Color Books given by the proposers and it was very incomplete. There was some doubt about the intention of the proposed project.

KHH reported about another project presented at the last Bureau meeting which aimed at establishing a data management system for all IUPAC publications. The task group leader in this project was D. Brynn Hibbert (President, Division V).

Apparently, however, there is only one project and it is primarily about the Green Book and the Gold Book. The output is primarily intended for database users. The project will to some extent take care of Gold Book inconsistencies. It was stated that one cannot have duplicate entries in the data management system. A new committee or similar body to deal with this should draw on people from various fields; GPM had stressed in ICTNS that all Divisions should be involved.

8.20 Nomenclature of Transition States and their Analogs for Phosphoryl Transfer Reactions (proposal 2013-039-1, Blackburn).

GPM pointed out that the project had been approved in September 2013 and was now project 2013-039-2-300.

GPM is a task group member and will go to a task group meeting in Malaga in November.

8.21 Protecting group abbreviations (the project was 2011-044-1-300).

There are errors in the published document [*Pure Appl. Chem.* **85**(1), 307–313 (2013)] and it probably needs to be republished.

RMH, GPM, and KHH will go through the document again and get back to AR.

9. Future projects/activities

9.1. International Organization for Standardization (ISO) liaison.

ATH told that EN was planning a scoping meeting on metal clusters in London in November after the RSC General Assembly. The result could be a project proposal.

It was suggested to keep contact with the boranes project (item 8.9) since there might be overlapping concepts or approaches.

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

[Secretary's note: On the IUPAC web site, Red Book project 1999-001-1-200 is mentioned under Division II and not under Division VIII – it was started in the old Commission on the Nomenclature of Inorganic Chemistry before Division VIII was created.]

It was discussed whether a new edition of the *Red Book* could be ready for the IUPAC centenary in 2019. RMH said we are in a way already working at it, developing the use of the kappa notation, looking at rules for the selection of central atoms, and in the boranes project. We would need to find solid state expertise. This could perhaps be done via ATH's contact to Division II (cf. item 7). Division II had had a young observer in Istanbul who might be interested in getting involved. TD said there are a number of errors in RB 2005 that should be corrected at the very least. RMH volunteered to shepherd the initiation of a revision.

9.3. Graphical representation of polymers.

This needs to be dealt with in the future!

9.4. Rotaxane stereochemistry.

AY and KHH had tried to recruit people, but potential task group members kept slipping away.

AY says there are unsolved and interesting problems that also concern other systems than rotaxanes.

9.5. Delocalised systems.

TD had not made any progress prior to the meeting, but mentioned that in a Blue Book discussion just the day before in Bangor, WHP had pointed to rules for choosing a parent anionic structure (Blue Book P-72.1) that could also be used for choosing in delocalized systems the particular resonance form on which to base the preferred name. Following these rules, acetylacetonate would get the preferred name 4-oxopent-2-en-2-olate rather than 2,4-dioxopentan-3-ide. This would solve the immediate problem of selecting a preferred name for the ligand acetylacetonato (*i.e.*, it would be 4-oxopent-2-en-2-olato).

There was probably still good reason to look at other delocalized systems. For this, it was suggested to go back to the 2004 Blue Book draft and see what was there and what had been eventually left out in the later version of the book. Contact should also be made to the relevant InChI subcommittee task group(s) dealing with delocalized systems.

AY pointed to the relation to the problems in naming tautomers and the possibility of setting up a project on this.

It was finally decided that AY and TD should work at scoping such a project or projects within a time frame of 6 months.

9.6. Crown nomenclature.

Already Charles Pedersen himself had noted that crown names are in principle ambiguous. AY said they can be named asphanes. KHH wanted to include calixarenes.

PH asked what is the need for new crown nomenclature; perhaps we should just have a technical report describing the various naming possibilities.

9.7. Central web page for all IUPAC recommendations/publications.

This idea was being considered by Roger Hiorns (chairman of the Division IV Subcommittee on Polymer Terminology) and KHH. It cannot be realised in the current situation with the IUPAC web site which is not fully functioning and not easily modified as is GPM's web site.

AY suggested we could have a separate division page and TD asked whether we could be given permission to edit such a page ourselves.

(See also item 13.3.)

9.8. Document on italic and roman fonts.

KHH wanted to make contact to Ron Weir, chairman of ICTNS, regarding this subject. An old document by Val Metanomski and Ian Mills was mentioned. GPM later gave the reference: http://old.iupac.org/standing/idcns/fonts_for_symbols.html.

Comments were made on what is in the Color Books. There would probably be a basis for a new project.

9.9. Other projects.

Class names with Div II and III (including bioinorganic). TD mentioned the old glossary on bioinorganic terms which needed attention.

ATH will make contact to people in the area of supramolecular chemistry (see Istanbul minute 9.9). There is a chapter on nomenclature in the series on supramolecular chemistry.

KHH mentioned polymeric carriers and glycoconjugates which often occur with drugs but also conjugates of drugs with proteins. GPM said the INN cannot be changed. He said linkers are a problem and mentioned PEGylation. KHH said the problem arose in the modified polymers document. GPM mentioned that there are also problems with dendrimers.

Index of Blue Book (cf. item 8.2): we could get inspiration from the index in the *Principles* book. Or maybe we could work at expanding the contents list.

Amine project (see item 8.2).

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

[Secretary's note: The minutes from Istanbul contain several more or less explicit action points of this kind under the corresponding item 10 there. Connected to item 9.7 above.]

IUPAC is not providing naming services as such, but there were now contact addresses for the Blue Book and for polymer nomenclature, and KHH was to ask the secretariat to establish an address for inorganic nomenclature as well.

11. Membership matters

11.1. Status of Division VIII Committee membership.

[The 2014–2015 roster as it looked at the time of the Bangor meeting is inserted here as Appendix A.]

KHH mentioned that Antony Williams wished to step down as titular member for personal reasons. It was agreed that the vacancy should be filled as soon as possible so as to have a good pool of titular members for the regular elections in 2015, where a new secretary must be elected.

Accordingly, steps would be taken to conduct with the secretariat a fast election procedure via E-mail of a replacement for AW.

Regarding eligibility for various positions in the coming biennium, KHH would send out a list of current Division members with information on completed terms of service.

See item 6a regarding the next election cycle.

11.2. Division VIII Committee representatives in other IUPAC bodies.

CCE – RMH.

Pure and Applied Chemistry Editorial Board – ATH. ATH noted that he had had no communications from the board since Istanbul.

ICTNS – AR is the Division VIII representative. GPM is also a Titular Member of ICTNS.

COCI – No official representative from Division VIII on COCI.

JCBN – TD, KHH, and AR are currently members of JCBN. GPM is the chairman of JCBN.

InChI Subcommittee – AY and HR are members.

11.3. Division VIII Advisory Subcommittee (ASC).

Since Istanbul, KHH had added the Istanbul observers to the ASC and the Discussion Board. ATH noted that the observers Markus Etzkorn and Ilia Guzai had expressed interest in becoming involved in the Division's work. However, we still needed to find out about their specific interests.

KHH noted that ASC member Alan Katritzky had passed away in February. The Division Committee stood for a moment in remembrance.

KHH/TD were to check the addresses of ASC members.

TD commented that we do not do enough to inform ASC about current projects. He was to send a message to the ASC about new projects.

12. Status of Division VIII web board with discussion forums

Towards the end of 2013, the membership of the Division Committee had been finally updated on the IUPAC web site.

There had been problems with the secretariat's updating of the memberships for the discussion forum in early 2014, but KHH declared that the forum was now working.

KHH had had no reply from Division VIII members from the preceding biennium whether they agree to stay members of the Advisory Subcommittee. There was a discussion of when to use E-mail and when to use the discussion board. No clear conclusion was reached. Currently the ASC forum does not send alert e-mails, so it is best to send important messages also by e-mail.

13. Publicity

13.1. Division VIII (and related) publications since the 2013 Division Committee meeting.

A list of publications is included as Appendix B. For details about the Blue Book: see item 8.2 above.

KHH mentioned the deplorable new situation with the restricted access to *Chemistry International*. [Note: Right after the return from the meeting, KHH became aware of three new German IUPAC translations by *Angew. Chem.* (see Appendix B).]

13.2. IUPAC-IUBMB nomenclature web site.

GPM did not have much to report. Due to a problem with the College computing system he was no longer able to get statistics on use of the nomenclature web site. He had had a problem correcting and updating the site early in 2014 but this was no longer a problem by August.

13.3. IUPAC web site.

There was agreement that the web site was not functioning well and was not set up in a user-friendly way. However, behind these problems were aspects of security and software compatibility across geographies.

KHH reminded about his message earlier in the year about the committee that had been set up to work at improving the web site. The committee had sent out a survey that was supposed to go also to the NAOs (TD to check whether that had actually happened, but the survey was now closed).

13.4. Quality of IUPAC output.

KHH warned against premature submission of documents; all comments submitted must be considered. There are IUPAC publications with glaring errors.

Ron Weir, the ICTNS chair, had stated clearly that "Having to print corrigenda is a process that must be avoided by getting it right in the beginning."

Public and ICTNS reviews now run in parallel. There is a problem in who does ICTNS assign as reviewers.

KHH reiterated the way to deal with definitions of terms. Publications are often not consistent with the *Gold Book*. GPM asked how broadly must terms agree.

It was mentioned that ICTNS hoped to initiate a project to update the Gold Book.

[Secretary's remark: cf. 8.19 above.]

14. Reports from other IUPAC bodies

ICTNS: GPM said there was very little to report.

JCBN: Several projects being worked at or planned under the auspices of JCBN have already been mentioned (see items 8.4, 8.6, 8.12 and 8.15 above). During the last year, 252 new enzyme entries had been added to the EC list; however, the rate of additions had leveled off.

It had been proposed to review the old electron-transport proteins document in a year's time.

The next meeting was planned to be in Braunschweig, Germany, on May 11–13, 2015.

CCE: There had been a meeting in Toronto in July. RMH had not been there but had asked for a brief report.

AY sent out a report on InChI for polymers half a year back.

A short discussion about the star indicating free valences in formulae used in publications vs. databases arose. AY said the star has been used for decades in databases and cannot be changed, but can be hidden in publications.

AY said it is a problem that there is not an established communication channel from InChI Subcommittee to Division VIII. In the future we should remember to request reports from the InChI Subcommittee and from the InChI projects.

[Secretary's remark: see item 8.1 about the unfortunate fall-out in the communication from the Division to the InChI Subcommittee.]

15. Any other business

Liaison to ACS: KHH had received a permanent invitation to participate in the meetings of the ACS Nomenclature Committee. However, at the next upcoming meeting, RSL would be our representative. WHP would participate in the spring meeting. GPM is a corresponding member of the Committee.

KHH repeated that task group leaders should keep him informed about work going on and forward draft documents as appropriate.

TD brought up again the problem that IUPAC is using a plethora of ill-defined terms to qualify its recommendations for usage of, and advice not to use, names or terms (*e.g.*, 'acceptable', 'recommended', 'approved', 'preferred', 'may be used', 'not recommended', 'not acceptable', 'discouraged', 'deprecated', 'not included in current recommendations', ...). He reiterated that according to a decision in the Division, in the graphical representation documents only three terms were to be defined and used: *acceptable*, *preferred* and

not acceptable, and he asked why we could not continue this practice. KHH remarked that we would have to agree with other Divisions, so that it would have to be a decision made via interaction with ICTNS. It was agreed that as a first step, TD should prepare a short document on the issue to be discussed in the Division before approaching ICTNS.

There had been uncertainty about the official project numbers for some of the joint projects between Division VIII and other bodies, cf. secretary's note under item 9.2. Was the numbering to reflect financial/funding aspects or responsibility for projects? TD was to contact Fabienne Meyers to find out about the numbering and the listing of the projects on the web site.

16. Dates and venue for next meeting

The dates of the IUPAC General Assembly in 2015 will be 6–13 August, and the venue will be Busan in South Korea. The IUPAC Congress will be 9–14 August.

The Division VIII Committee meeting will be around the weekend 8–9 August.

Task group meetings may or may not be at the same venue. But we should make sure that task groups are not let alone in arranging for a suitable venue.

17. Adjournment

KHH once again thanked MAB and thanked everybody in attendance for their participation.

Appendix A

Division VIII, membership roster for the biennium 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. Ebbe Nordlander	TM	2014-2015	Sweden
Prof. Amélia Pilar Rauter	TM	2014-2015	Portugal
Dr. Hinnerk Rey	TM	2014-2015	Germany
Dr. Antony Williams*)	TM	2014-2015	United States
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. Risto Laitinen	NR	2014-2015	Finland
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
Dr. Gerard P. Moss	<i>Ex Officio</i>	2014-2015	United Kingdom

*) Stepped down after the Bangor meeting. A new TM will be elected. See item 11.1.

Appendix B

IUPAC Publications since the Division VIII Committee meeting in Istanbul in 2013

The list contains publications issued under the auspices of the Division and other material of interest to the Division.

Blue Book:

IUPAC; H. A. Favre, W. H. Powell (Eds.): *Nomenclature of Organic Chemistry – IUPAC Recommendations and Preferred Names 2013*; xliii + 1568 pp., Royal Society of Chemistry, Cambridge, UK, 2014

Purple Book:

www.iupac.org/fileadmin/user_upload/publications/e-resources/ONLINE-IUPAC-PB2-Online-June2014.pdf

Other publications

G. J. Leigh, Polymer Nomenclature, *Chem. Int.* **35**(4), 25–26 (2013)

G. J. Leigh, The Special Case of Boron Hydrides, *Chem. Int.* **35**(5), 24–25 (2013)

G. J. Leigh, Use of Abbreviations, Enclosing Marks, and Line-Breaks, *Chem. Int.* **35**(6), 24–25 (2013)

A. Yerin, A. McNaught, S. Heller, InChI – the IUPAC International Chemical Identifier, *Chem. Int.* **35**(6), 12–15 (2013)

B. F. Thomton, S. C. Burdette, Naming Superheavy Halogen and Noble Elements, *Chem. Int.* **35**(6), 26–27 (2013)

R. Bucat, Visualization, Mental Models, and the "Reality", *Chem. Int.* **36**(1), 9–13 (2014)

J. Meija, Symbols of the Elements, *Chem. Int.* **36**(1), 20–21 (2014)

In Memoriam: Henri A. Favre 1926 – 2013, *Chem. Int.* **36**(2), 17–18 (2014)

J. Meija, Symbols of the Elements, Part II, *Chem. Int.* **36**(3), 18–20 (2014)

J. Meija, Symbols of the Elements, Part III (concluded), *Chem. Int.* **36**(4), 25–26 (2014)

E. Scerri, On the Naming and Symbols of Elements 115 and 112, *Chem. Int.* **36**(4), 26–27 (2014)

New Edition of the "IUPAC Blue Book" Nomenclature of Organic Chemistry – IUPAC Recommendations and Preferred Names 2013, *Chem. Int.* **36**(4), 22 (2014)

Terminology of Metal-Organic Frameworks and Coordination Polymers, *Pure Appl. Chem.* **85**(8), 1715–1724 (2013)

Abbreviations of polymer names and guidelines for abbreviating polymer names (IUPAC Recommendations 2014), *Pure Appl. Chem.* **86**(6), 1003–1015 (2014)

Translations of IUPAC Recommendations and Technical Reports into German

(Update by KHH August 21, 2014)

The journal *Angewandte Chemie* (*Angew. Chem.*) since 2002 has been publishing translations of IUPAC Recommendations and Technical Reports into German. 32 translations were published from 2002 through 2010. In addition, one of the translations has been republished in a revised version in 2011. After an interruption in 2012 and 2013, three further translations have been published in 2014.

Of relevance to Division VIII is the translation of the "Terminology of metal-organic frameworks and coordination polymers".

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 C

InChI Subcommittee report to Division VIII July 2014

Summary

Since the February 2014 report there continues to be good progress with InChI and the InChI Trust in a number of areas. A new project proposal for large/biological molecules has been approved by IUPAC. In addition another new working group for positional isomers has been formed. Publicity for the project remains very good and has resulted in considerable increase in the uptake and usage of the InChI algorithm. The InChI Symposium at the ACS meeting has been scheduled as two half-day sessions; one each on Sunday and Monday. The FDA has chosen to join the Trust. Lastly, the InChI team was awarded the Chemical Structure Association (CSA) Mike Lynch Award.

Items covered in this report

Membership/Support

InChI RFP/Contracts

IUPAC InChI Subcommittee and working parties/groups

Meetings attended & talks/posters given

Manuscripts & other publications

InChI Trust web site

InChI Usage

Technical issues

Plans for 2014

Membership/Support

Summary: A number of organizations are still in the process of joining or talking about joining, but there still is little progress. Like most organizations, since InChI works and it is not high on their immediate priority lists, actual real progress is slow.

As of July 18, 2014

Existing Members and Associates: 14 – FDA has joined.

Supporters: 46

Certification Suite purchases: 2 – NCI and Novartis – in process

InChI RFP/Contracts

The contract for Markush structures with Digital Chemistry remains on hold awaiting potential funding.

A contract for taking the RInChI work that Jonathan Goodman and Chad Allen did at Cambridge University is expected to be signed by the fall of 2014.

A contract with Jeremy Frey to develop a proof of concept for developing an app for InChI QR codes is underway. The initial results will be reported at the ACS San Francisco InChI Symposium.

A contract for an InChI Trust web site in the cloud is underway and expected by fall 2014.

IUPAC InChI Subcommittee working groups

Positional isomers

Considerable interest in positional isomers has developed in the past few months. Chris Steinbeck at EBI has agreed to chair the working group for this effort. This is background for this working group that Chris has drafted:

There is a need for a canonical representation to encode positional isomers of (bio-)organic molecules. Use cases include the concise representation of positional isomers that were either systematically synthesized or isolated from a biological system.

Depending on the amount of evidence available, the identification of (bio-)organic molecules can also be ambiguous, in which case one will want to represent a number of possibilities for true identity of the partially identified compound.

This working group will produce a specification for the extension of the IUPAC InChI to allow for the canonical encoding of positional isomers. To this end, it will gather user requirements from a number of subspaces of the applicable chemistry community and ensure that the specifications are in line with the strategic value to IUPAC.

The white paper with the specifications will be discussed with experts from the InChI trust and prototypes will be produced, tested and refined in an agile development process.

Chris has put together the following experts from 5 countries as members for his working group:

Christoph Steinbeck, Chair
Egon Willighagen
John May
Steffen Neumann
Steve.Stein@nist.gov
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. A status report is expected to be available for the Trust San Francisco meeting.

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 2014. Igor will report on this at the Trust San Francisco meeting.

Reactions

Guenter Grethe has been unable to move forward with his working group owing to the lack of a contract to clean up and do further testing of the current software. With the expectation that a contract will be signed by the fall of 2014 this project should again be moving forward.

009-043-2-800 Standard InChI-based Representation of Chemical Reactions

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

Chairman: Grethe, Gunther

Members:

Batchelor, Colin
Goodman, Jonathan
Kraut, Hans
Lawson, Alexander
Schmidt, Martin

Markush

We are still waiting for the needed financial support before proceeding. David Evans plans to discuss this matter in some detail at the Board meeting.

Electronic States

Don Burgess at NIST has developed two draft plans (available upon request) for InChI for Representations of Species at the Molecular Level. Don will give a talk on this at the InChI symposium in San Francisco in August.

InChI for Materials

No news from the NIST staff about this.

Organometallics

Colin Batchelor and his working group expect a final report by the fall of 2014.

Inorganics

Hinnerk Rey from Elsevier/Frankfurt has replaced Nigel Wheatley to head up this working group. His 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](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2012-046-2-800)

Chairman: Rey, Hinnerk

Members:

Damhus, Ture
Druckenbrodt, Christian
Hartshorn, Richard
Schenk, Roger
Sitzmann, Markus

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

Keith Taylor, who has just been retired at Accelrys, had his proposal to IUPAC approved in October 2013. The work will be based on the work he has done at Accelrys and has made publicly available. The Pistoia HELM project, while lacking a number of technical capabilities (*e.g.*, it does not support variably attached drugs or variable groups and it has limited canonicalization), is moving forward. There are many issues with the project, which seem to be ignored by those running the project. There is no one responsible for any bug fixes. Major changes will be done by sending out a RFP. Those at Pfizer who developed HELM have been let go or reassigned, but seem to be involved without management knowledge. How this can function, let alone become a real standard, is beyond me. They have expressed no interest in working with IUPAC or the InChI Trust. Keith, Evan Bolton (NIH), and I remain on the HELM mailing list to monitor what is going on.

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

Chairman: Taylor, Keith

Members:

Blanke, Gerd
Bolton, Evan
Chalon, Didier

Drijver, Alex
Jensen, Jan
Yerin, Andrey
Helen Berman

The first meeting of this working group will be held at NIH on October 27 & 28, 2014. The meeting is to be sponsored and hosted by NLM/NCBI, but they are providing no financial support – only the meeting room space. There will be no registration fee for anyone who wishes to attend.. This will be a two-day meeting with short presentations the first morning by a superb set of speakers with knowledge and experience in the area:

Philip Bourne, NIH Associate Director for Data Science
Helen Berman, IUBMB & PDB, Rutgers
Keith Taylor, Working Group Chair
Evan Bolton, PubChem
FDA (Larry Callahan or Yulia Borodina)
NIH/NCATS (Tyler Peryea)
EBI (Sameer Verlanker)
Roger Sayle (nextmovesoftware)
HELM (Sergio Rotstein)
BIOVIA (Matt Sage)

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 held his first working group meeting at the ACS New Orleans 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](http://www.iupac.org/nc/home/projects/project-db/project-details.html?tx_wfqbe_pi1[project_nr]=2012-023-2-800)

Chairman: Nicklaus, Marc

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.

January 2014 – August 2014 activities

Meetings attended; talks/posters presented

I gave an InChI talk at the BioIT InChI workshop in April. About 10 people paid to attend.

Other speakers included Tony Williams, Steve Boyer, Chris Southan, and Evan Bolton.

I gave an InChI presentation at the APHL (Association of Public Health Laboratories) in April. About 40 people attended.

I gave two InChI seminars in Singapore at the NUS and NTU universities on May 15 and 16. About a dozen people attended each talk.

I gave three presentations at the July meeting in Toronto, which included a formal talk and a workshop presentation on how to create InChIs. I was invited to these sessions by Bob Belford, who is trying very hard to get more university and other teaching staff to incorporate InChI in their teachings.

On behalf of the entire InChI team I gave the CSA Mike Lynch Trust award talk at the 10th ICCS meeting in Noordwijkerhout in June. The five InChI team members (below in alphabetical order) were given the Mike Lynch award for the work on developing InChI:

Steve Heller
Alan McNaught
Igor Pletnev
Steve Stein
Dmitrii Tchekhovskoi

Manuscripts

No additional manuscripts were published by the InChI team.

Igor expects to have his manuscript ready by the ACS meeting in San Francisco.

Other publications

As a result of the InChI poster (co-authored by the folks at LSU) given at SLA 2013 in San Diego in June, I was asked by the journal editor, Tony Stankus, to prepare a paper for publication in the “Science & Technology Libraries” journal. To be sure this paper is sufficiently and appropriately different from those already written by myself, Alan McNaught and others, I have asked Bill Armstrong at LSU to take the lead in writing this paper. So far Bill has still not gotten very far with preparing the manuscript in spite of a number of reminders.

InChI Trust web site

The Trust web site is now up on the IUPAC server. There have been a number of problems with the web site and plans are underway to move to the cloud. Aletia Rey has been hired to maintain and add content to the web site.

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.

In February 2014 the ACS *J.Med.Chem.* came out with an editorial encouraging authors to submit SMILES as structure representation for molecules in their manuscripts.

<http://pubs.acs.org/doi/abs/10.1021/jm5002056>

In a series of conversations – public on the CINF list and in private – were unable to get the Journal to alter its current plan and add InChIs and InChIKeys. The main concern seems to be that converting an InChI string back to a structure does not give a pretty as picture and accurate picture as the author might wish. Since the drawing is actually a function of the structure drawing programs, not SMILES or InChI, this continues to puzzle me. Specifically they said (in an email): “Our major concern when adding a line notation representation of chemical structures to JMC articles was to faithfully reproduce the structures drawn in the data tables in the paper”. The fact that SMILES are not unique (as pointed out in the case of Warfarin that Marc Nicklaus found on the web) does not seem to have bothered these people. I referred to this approach as “art” vs. “science”. Also they believe, against all evidence, that authors will do what they wish and there is

no need for the publisher to get involved. At the same time they admit the publisher has shown no interest in helping. Lastly, since I was told any SMILES entered in the manuscript will be supplemental information, I was told it will not be searchable. While we were not able to change anything at this time, virtually every response to the CINF list was in support of InChI and not SMILES. So, at least, we came out of this looking very good.

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 2014

For the remainder of 2014 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. Help to organize the InChI Large Molecules meeting at NIH/NLM/NCBI in October 2014.

Steve Heller, Chair

Alan McNaught, Secretary