

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

***Minutes of Division Committee Meeting
Istanbul, 9–10 August, 2013***

1. Welcome, introductory remarks and housekeeping announcements

The President of the Division, Richard Hartshorn, welcomed members and observers to the meeting and thanked Alan Hutton for agreeing to take the minutes of the meeting in the absence of the Division Secretary, Ture Damhus. The committee asked that its greetings and best wishes for a rapid recovery to full health be conveyed to Ture.

The meeting stood in silent remembrance of three eminent IUPAC nomenclaturists who had passed away in the preceding year: Henri Favre, Herb Kaesz and József Nyitrai.

The President briefed the meeting on visits that would occur that afternoon from representatives of CCE and COCI, as well as on the inter-Division cross-over sessions that would be held the next day, asking members to think up appropriate topics for discussion at those meetings [*see minute 7. later and Appendix B*].

2. Attendance

Present: Richard Hartshorn (President; RMH), Karl-Heinz Hellwich (Vice-President; KHH), Michael Beckett (MB), Philip Hodge (PH), Alan Hutton (ATH), Gerry Moss (*ex officio* – JCBN; GM), Ebbe Nordlander (EN), Warren Powell (WHP), Amélia Rauter (AR), Jan Reedijk (from late afternoon of Day 1, sharing time with Div II; JR), Hinnerk Rey (HR), Andrey Yerin (AY).

Observers: Ronald Castellano (for item 17 on Day 2 only, USA; RC), Markus Etzkorn (USA; ME), Ilia Guzei (USA; IG), Saleh Khamlich (South Africa; SK), Alain Krief (from Day 2, International Organization for Chemical Sciences in Development, IOCD; AK), Daniel Lowe (NextMove Software Ltd, Cambridge, UK; DL), Wandee Luesaiwong (Thailand; WL),

Apologies: Ture Damhus (TD), Md. Abul Hashem, Gernot Eller, Jaroslav Kahovec.

No message received: Vefa Ahsen, Itrat Anis, Sundarababu Baskaran, Kirill Degtyarenko, Wei Huang, Lupituko Luko Mkyayula, József Nagy, Supawan Tantayanon, Nigel Wheatley, Antony Williams, Jeff Wilson.

3. Introduction of attendees

RMH invited the attendees to introduce themselves around the table.

4. Approval of agenda

RMH pointed out that some items might have to be switched around to accommodate visits from other committees and inter-divisional cross-over sessions; otherwise the agenda was approved.

5. Approval of minutes of meeting in Lisbon, Portugal, 2-3 July 2012

The latest draft (dated July 29) had been circulated via e-mail with the agenda for the present meeting. The minutes were formally accepted *nem. con.*, with corrections noted to minute 2 (correct spelling 'Vefa Ahsen') and minute 9.1 (word 'new' repeated twice in 2nd sentence). Note also comments under item 6 below.

6. Matters arising

It was pointed out by GM and KHH, in relation to Lisbon minute 6 (which itself referred to San Juan minute 9.2), that KHH's statement regarding the name 'acetylamino' was correctly minuted, but the statement was wrong because the carbohydrate document uses the name 'acetamido'.

With reference to Lisbon minute 13.1 it was noted that the Russian translation of the Blue Book was on hold for financial reasons.

At this point the President, RMH, reported on his briefing with the Secretary General, René Deplanque:

- (a) John Petersen had resigned as manager of the IUPAC Secretariat and Terry Renner temporarily had stepped in instead of John Petersen.
- (b) The IUPAC servers had been hacked and had now been moved to Research Triangle Park in North Carolina, the move being necessitated by the sale of FIZ Chemie to Wiley. An advantage was that Bryan Pearson would now have full access for updating records, *etc.* RMH said the Division should take advantage of the move to engage with Bryan in order to show our nomenclature activities to a wider world. Several committee members voiced their criticism of the IUPAC website, highlighting, for example, its lack of search facilities. AY volunteered to collate a list of complaints and engage with Bryan. RMH requested the committee to send comments to AY, warning, however, that the website is now a small operation and run by one person. [*See also minute 12.*]
- (c) RMH reported that Hugh Burrows (Portugal) had been appointed to succeed James Bull as the new Editor of *Pure and Applied Chemistry*. As a result of the poor state of the finances of IUPAC's publishing endeavours, a decision had been taken to outsource publication of PAC and *Chemistry International* to a commercial firm, namely De Gruyter. Indeed, the reduction of Division VIII's budget from USD 80 000 to USD 70 400 was partly a result of loss of income from PAC subscriptions.
- (d) RMH relayed to the committee the Secretary General's desire to market IUPAC better and promote the brand strongly, mainly by cooperation with other organizations and by selling an IUPAC 'seal of approval'. Part of this would be to push for higher standards of publishing, using IUPAC standards of nomenclature and terminology; this would require appropriate processes, controls and auditing.
- (e) In discussion the committee took the view that journal and book editors no longer care about nomenclature and accept whatever authors use, relying on the referees of papers for approval, even though comment on the nomenclature used was rarely specifically asked of referees. It was noted that many students use ChemDraw to name organic compounds and that coordination and organometallic compounds, where additive nomenclature is employed, were still problematic. There was some discussion around the automatic naming of compounds, and ME enquired whether IUPAC provided any service to help authors name compounds. It was proposed and agreed that the experiences of people using various naming programs be recorded and that AY creates an IUPAC webpage with information on the programs, books and documents available to authors, students and others. RMH warned that care should be taken not to endorse particular non-IUPAC products. It was noted that the new series of 'Essentials' brochures will help, and some thought was required as to the best way of disseminating these to editors and authors. [*See also minute 10.*]

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

Under this item the committee prepared, in a teatime breakaway session, for the interdivisional cross-over meetings to be held on the following day. After some discussion around what might be expected from these meetings it was decided that AY would lead the discussion with Division I, MB the discussion with Division II, GM the discussion with Division III, and KHH the discussion with Division IV. [*A report on these meetings may be found in Appendix B.*]

8. Updates on Division VIII projects

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

As a general point, RMH requested all Task Group Chairs to update project information on the IUPAC website.

HR gave a general survey of the state of each of the InChI-related projects, reporting that the new projects on 'Handling of inorganic compounds for InChI V2' (2012-046-2-800) and on 'Redesign of handling of tautomerism for InChI V2' (2012-023-2-800) had been approved and were on stream. The project on 'Implementation of InChI for large molecules' (2013-010-1) was thought to be still awaiting approval and Keith Taylor was responsible. No progress was reported for the project on 'InChI requirements for representation of organometallic and coordination compound structures' (2009-040-2-800). AY made a plea for the InChI Polymers project to be completed as soon as possible. HR highlighted that the output of all of these projects is a set of rules and algorithms on how to process compounds for communication between machines rather than between humans. Several committee members commented on the five really excellent YouTube videos describing the InChI concept that may be found at <http://www.youtube.com/user/InChITrust>.

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

Reporting on the status of the Blue Book, WHP said the entire 1576-page camera-ready manuscript would be ready for submission to the RSC at the end of the month (August 2013), in which case the RSC had indicated the book could be published before the end of 2013. WHP then briefly summarized the history of the project, emphasizing the important contribution of Henri Favre, who came up with the idea of preferred names in 1993. WHP had joined the group in 1998, and today the project was complete, mainly due to the persistence of Henri. The manuscript had been reviewed in 2004 and 2010, and adjustments made as appropriate. Appendix 2 (a 60-page table of detachable prefixes) still needed to be edited and reviewed, a task Henri was in the midst of when he passed away. AY and GM had since helped out with this task, and now only minor inconsistencies needed to be addressed. Marcus Ennis had done an editorial review of the manuscript and approval had been received from Ron Weir (ICTNS). In July 2013 WHP had been in communication with Janet Freshwater of the RSC concerning how the index to the book was going to be done. WHP had understood the RSC would compile the index, but it was not clear whether this was in the contract with the RSC. WHP was going to discuss this further with Sara Bowler from the RSC, who was present in Istanbul, on Monday 12 August.

KHH noted two changes since the 2010 review that should appear in the list of changes, one concerning chromene (benzopyran), the other concerning a recent possible alternative numbering for chalcone requested by the flavonoids task group. It was agreed that KHH, GM and WHP would get together to resolve these issues and report back.

The discussion concluded with RMH observing that a 1576-page document was never going to be error-free and should now be published as soon as possible. The committee endorsed this sentiment, and WHP was congratulated and thanked for his indefatigable efforts in this Herculean task.

[*See also minute 15.3.3.*]

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

No progress reported.

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

No progress reported. GM indicated that this and the previous project [*see minute 8.3*] were on his desk, and just needed activation. RMH urged that progress be made with these projects, and as a general point encouraged task group leaders to move forward yearly with their projects.

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 summarized progress from the meeting held the previous day. Good progress had been made, and publication could be expected before not too long. Unfortunately Jonathan Brecher and Arthur Maximenko had been lost to the project team, but there was the possibility of Jörg Pabel joining the group.

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

AR described the good progress made by the large group involved and reported on a recently held meeting.

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

RMH reported that there had been slow but positive progress. The first task, that of describing the kappa convention, had turned out to be more extensive than initially envisaged. There were drafts of several documents in progress; the idea was to publish first the kappa grammar recommendations, then a separate document on the selection of a central atom. That would be followed by a list of retained names, *e.g.*, of simple salts, which would need to be curated. Finally, there should be an overarching document defining the procedure to go through to arrive at a PIN.

There was still a need to address PINs for organometallic compounds, *e.g.*, methyl vs. methanido, and how to separate ligands from the central atom. RMH mentioned that WHP had mooted a possible alternative way of naming ligands in which the characteristic group is moved to the top of the priority list when it coordinates. This would provide different names for coordinated ligands compared with free ligands.

AT THIS POINT THE MEETING ADJOURNED FOR LUNCH

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

The organic group had a meeting and some changes had been made to the extant document, thanks to AY. The inorganic document had been circulated to the Division Committee and comments were welcomed. RMH described the documents as a 'distillation' of current nomenclature. Publication of the documents would be as Technical Reports, followed by dissemination to editors, textbook authors, as a pull-out in *Chemistry International*, etc. A date of 16 Sept 2013 was set for review feedback.

[*Appendix C contains a detailed list of all re-publications of the 'Brief Guide to Polymer Nomenclature' supplied by Roger Hiorns, which should prove useful in deciding how to disseminate the inorganic and organic counterparts.*]

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

This project had been approved earlier in the year, under MB's leadership, with four Division Committee members and four external experts. MB reported that the first meeting of the group would take place during the current General Assembly on 11 August. The project would be presented as a poster at the EuroBoron VI conference in September 2013 by MB.

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

GM reported that the intention was to produce an interim document that could be used to apply for further funding for the third part of the project. There should be a first draft by the end of the year.

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

ATH reported that this project, which had been in gestation for some time, had very recently been approved, and in record time from submission, so that the first meeting could be held at the current General Assembly in two days' time, on 11 August. He thanked the officers concerned for the speedy passage of the project application through the assessment process leading to its approval.

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

AR reported that the project was nearly finished and that a manuscript would shortly be submitted, after initial review by the Division Committee.

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

This is a project with Division II, led by Lars Öhrström. There was a document in the system for publication, currently in the public review stage. AY and KHH were not happy with some of the names used in this document, though the document is about terminology and not nomenclature. Further enquiries would be made at the cross-over session to be held with Division II the next day.

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

KHH reported that this project sought to revise an old document from 1984 and was a collaboration among Divisions II, IV and VIII. There was no further information on progress, but a meeting was scheduled for 12 August at the current General Assembly.

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

GM reported that this was basically a JCBN document and that the project 'struggles on'. The database does not exist. The original objective was to deal with compounds not covered by other reference sources and GM felt that perhaps the project may be going somewhat off track. Something publishable was needed, and RMH agreed to write to the chair, Richard Cammack, to establish the current status.

8.16. Polymer projects (with Division IV)

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

KHH reported that this project had been in existence for 10 years now, and that Richard Jones was trying to get it finished. Certainly the document is improving all the time and there would be a meeting at the current General Assembly in two days' time.

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

Richard Jones had taken control of this project and there had been two new drafts in the last year. KHH had sent comments to Richard Jones and there would be a meeting in Istanbul in two days' time.

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

This was a problematic document and the leadership of the project had changed several times. However, a document had been submitted for review in the previous week.

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)

Werner Mormann and KHH had been working on this document. There would be a meeting in Istanbul in three days' time.

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 reported that this project had been 90% complete for two or three years. The 25-page document was now close to completion and there would be a meeting in Istanbul in three days' time.

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

There was no news on this project.

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

The document emanating from this project had been through the review process, and publication was imminent, pending a check of the extended list of abbreviations in the appendix by KHH.

8.16.8. Structure-based nomenclature for regular star and brush polymers (2013-031-2) (project proposal under review)

This project was under review – the task group was considered too small and the proposal had been sent back for modification and resubmission.

9. Future projects/activities

9.1. International Standards Organization (ISO) liaison

RMH had been liaising with the ISO joint working group on nanomaterials. The reason for this interaction is that ISO needs nomenclature to name nanomaterials. It was considered that nomenclature for carbon nanotubes and metal clusters might be feasible to pursue as joint projects. From their side, the ISO working group had vetted and recommended certain people for suitability to join nomenclature projects. From the IUPAC side, AY had been approached to take the lead in a project on carbon nanotubes, while EN would coordinate a metal cluster project in collaboration with ATH, ME and SK. Andreas Dress was mentioned as someone who might get involved at a later stage if a mathematical approach was required. Both projects should be considered to be preliminary and scoping in nature – was there any prospect of a useful nomenclature developing?

A caveat was that ISO would not provide any funding for these joint projects, all the funding would have to come from the IUPAC side. [See also item 15.1 on the agenda.]

[Note added in August 2014: ATH mentioned that the metal cluster group had proposed a scoping meeting in London in week 46, 2014, with additional participants Yasir Sultan and Eric Gulliver.]

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

RMH said the last edition of the 'Red Book' was seven years in the making. The centenary of IUPAC would be celebrated in 2019 and this would be a suitable occasion to publish an updated edition of the 'Red Book'. He asked for expressions of interest from those interested in joining a task group.

9.3. Graphical representation of polymers

KHH explained that this would be a different project from that on 'modified polymers' mentioned earlier [see minute 8.16.2.].

9.4. Rotaxane stereochemistry

AY reported that there had been no move forward with this potential project as no suitable task group members had been willing to be recruited. Also the Division had a smaller budget now and perhaps this was not a priority.

9.5. Delocalised systems

This was a potential project championed by TD and there was no news to report.

9.6. Crown nomenclature

KHH wondered whether calixarenes should be part of a project on crown nomenclature; otherwise there was nothing to report.

9.7. Central webpage for all IUPAC recommendations/publications

While it was acknowledged that the IUPAC website needs an urgent and complete revamp, the committee considered the idea of a central webpage for all IUPAC recommendations and publications highly desirable. The best option at the moment is GM's website at <http://www.chem.qmul.ac.uk/iupac>.

9.8. Document on italic and roman fonts

It was pointed out that an existing document dwelt more on the use of italic and roman fonts in physical chemistry, and that the intention here was to extend recommendations for usage in the realm of nomenclature. To revise the existing document would, of course, need ICTNS approval. Examples would be to consider what prefixes should be italicized, because there are consequences for how names are indexed and for using upper or lower case at the beginning of sentences. The relevant information in the 'Blue Book' and 'Red Book' could be merged to provide something like what appears in the introductory chapter of 'A Guide to IUPAC Nomenclature of Organic Compounds'. The possibilities of a project should be discussed further with Division I at the cross-over session on the next day's agenda. GM, ATH and possibly KHH expressed interest in this project.

9.9. Other projects

ATH pointed out that supramolecular chemists use symbols like Θ or \subset to indicate guest molecules in the formulas of inclusion compounds, and wondered if there might be a useful project in this area. No decision was taken.

AT THIS POINT THE MEETING ADJOURNED FOR AFTERNOON TEA

10. IUPAC expert nomenclaturists: suggestion submitted by Alexander Senning

The proposal from Alexander Senning to have a paid panel of nomenclature experts available to name compounds for clients was discussed. There was clear concern in the committee regarding the possibility of litigation if mistakes were made, so matters about legal liability and insurance would have to be fully investigated. KHH proposed that a consultancy or advisory service be provided rather than a direct naming service. At the Lisbon Division Committee meeting TD had been tasked to bounce the proposal back to Senning for further elaboration on the pros and cons. It was decided to hold over the discussion until the next day, when Senning's reply will have been seen.

[This discussion continued at the commencement of Day 2, but the minute is recorded here for convenience.] Senning's response was considered, and the question was raised whether CAS had insurance to cover legal liability in the case that incorrect names resulted in litigation. [After the meeting, as an example, AY provided information on how client service works at CAS. The terms and conditions (liability, *etc.*) for any CAS services rendered may be found at <http://www.cas.org/products/other-cas-products/client-services>.] AY maintained that IUPAC needed a 'PO Box' for enquiries, perhaps a standard e-mail address that could be used for all questions of nomenclature. According to AY, ACD had tried this, but they never received many

enquiries. Perhaps something more general than a naming service was needed; certainly a contact link should appear on the webpage. It was felt that this should be discussed at a general level for all Divisions. ME proposed that the Division rather make resources available on the website, better organized and with easier access than at present, and that there be a specific e-mail address given for advice on nomenclature matters. The Division would need to work to develop one or more appropriate contact points. The committee voted on this proposal and it was carried *nem. con.* [See also minute 6(e).]

11. Membership matters

11.1. Status of Division VIII Committee membership

For the 2014–2015 membership roster, see Appendix A. There had been very few participants in the voting due to the unclear instructions. Ten Titular Members were named, as well as six Associate Members. Nominations had been received for a total of 10 National Representatives, including Gernot Eller (Austria). Risto Laitinen would be invited to become an NR. RMH reported that TD had indicated his desire, if possible, not to continue as Secretary for his full term. RMH requested the Division's TMs to consider taking on this office for the new biennium and to indicate their interest to himself or KHH.

11.2. Division VIII representatives in other IUPAC bodies

The following holds for the next biennium:

CCE – RMH agreed to continue.

PAC Board – ATH agreed to take over from RMH and attend in Istanbul as an observer.

ICTNS – AR would be the Division VIII representative. It was noted that GM was also a Titular Member of ICTNS.

COCI – KHH informed the meeting that there was no official representative from Division VIII on COCI.

JCBN – TD, KHH, and AR were the representatives from Division VIII. GM as the chairman of both JCBN and NC-IUBMB is an ex officio member of the Division VIII Committee.

11.3. Division VIII Advisory Subcommittee

The list of members of the Advisory Subcommittee needs to be revised and updated. This body forms an electorate for the Division Committee and provides review and comment on Division documents. Anyone interested and willing to serve can join the Advisory Subcommittee. It is important to add new names, *e.g.*, of those who might become future Division Committee members. KHH will rationalize the list.

AT THIS POINT REPRESENTATIVES FROM CCE AND COCI ARRIVED, AND THE FORMAL AGENDA WAS SUSPENDED WHILE INTERACTION WITH THESE REPRESENTATIVES TOOK PLACE.

The delegation from CCE comprised the President, Mei-Hung Chiu, the Secretary, Jan Apotheker, and an observer, Mary Garson (Vice-President of Division III). Mei-Hung Chiu described some of the CCE projects and went on to say that her Committee was looking for sustainable, collaborative projects to promote chemical education. RMH described Division VIII's current 'Essentials' project, which provides a succinct distillation of the nomenclature of inorganic and organic compounds. RMH proposed that he brings this project to the forthcoming CCE meeting in Istanbul to invite comments and, specifically, to see if CCE can help with dissemination. A suggestion from PH was to produce YouTube videos on nomenclature similar to the ones produced by the InChI group [see minute 8.1. above].

The Chair of COCI, Michael Dröscher, spoke briefly about the functions of COCI and then invited all to join the WCLM (World Chemistry Leadership Meeting) with the 40 Young Observers on the afternoon of Tuesday 13 August at the General Assembly. He also spoke about the Safety Training Programme to take place on the morning of 14 August, and concluded with a request for all to ask their National Adhering Organizations (NAOs) how to improve interaction with COCI – his Committee needed the contacts and to get new people on board. KHH appealed for people from industry to read the 'Essentials' documents: once

finalized, Division VIII will send these to COCI with a view to their distributing them to companies world-wide.

THIS BROUGHT THE PROCEEDINGS FOR DAY 1 TO A CLOSE, AND THE MEETING ADJOURNED AT 5.00 PM.

[Day 2 started with continued discussion from the previous day on the proposal from Alexander Senning to have a remunerated panel of nomenclature experts available to name compounds for clients. This discussion is reported under minute 10. (above).]

12. Status on Division VIII web board with discussion forums

See minute 6.(b) for prior discussion on the IUPAC website. As far as the web board was concerned, the general consensus was that communication via e-mail seemed to be used in preference to the web board, which was not used as much as it should be. The facility is there, and members should feel free to use it whenever needed.

KHH noted that he was updating the membership list now, rather than waiting for the start of the new biennium, so that incoming members could have some overlap with communications. KHH would write a welcoming message to incoming members informing them that they were on the e-mail and web board lists.

13. Publicity

13.1. Division VIII (and related) publications since the 2012 Division Committee meeting

KHH noted that *Angewandte Chemie* had stopped publishing IUPAC documents translated into German.

The following publications were noted as listed in the agenda, no others being offered at the meeting:

Terminology and nomenclature for macromolecular rotaxanes and pseudorotaxanes (IUPAC Recommendations 2012), *Pure Appl. Chem.* **84**(10), 2135–2165 (2012).

A brief guide to polymer nomenclature (IUPAC Technical Report), *Pure Appl. Chem.* **84**(10), 2167–2169 (2012); also included as a two-page tear-out in *Chem. Int.* **34**(6) (2012); republished in *Polym. Adv. Technol.* **24**(1), i– ii (2013) and *Colloid Polym. Sci.* **291**, 457–458 (2013).

M. A. Brimble, D. StC. Black, R. M. Hartshorn, A. P. Rauter, C.-K. Sha and L. K. Sydnes, Rules for abbreviation of protecting groups (IUPAC Technical Report), *Pure Appl. Chem.* **85**(1), 307–313 (2013).

G. J. Leigh, What is IUPAC Nomenclature? *Chem. Int.* **34**(2), 24 (2012).

G. J. Leigh, On the Various Nomenclature Systems, *Chem. Int.* **34**(3), 28 (2012).

G. J. Leigh, Non-IUPAC Nomenclature Systems, *Chem. Int.* **34**(4), 27–31 (2012).

G. J. Leigh, Systematic and Trivial Nomenclature, *Chem. Int.* **34**(5), 28 (2012).

G. J. Leigh, InChIs and Registry Numbers, *Chem. Int.* **34**(6), 23 (2012).

G. J. Leigh, Deciphering and Constructing Names, *Chem. Int.* **35**(1), 21 (2013).

G. J. Leigh, Drawing Chemical Structures, *Chem. Int.* **35**(2), 26–27 (2013).

G. J. Leigh, Organometallic Nomenclature, *Chem. Int.* **35**(3), 27–28 (2013).

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

R. M. Hartshorn and H. Schepers, What's in a Name? Possibly Death and Taxes! *Chem. Int.* **34**(6), 29–32 (2012).

B. Herold, Lost in Nomenclature Translation, *Chem. Int.* **35**(3), 12–15 (2013).

Subsequent to the meeting, notice of the following publication was received:

M. Baron, K.-H. Hellwich, M. Hess, K. Horie, A. D. Jenkins, J. Kahovec, P. Kratochvil, W. V. Metanomski, W. Mormann, R. F. T. Stepto, J. Vohlidal and E. S. Wilks, *Kemija u Industriji*, **61**(3), 145–176 (2012). This is the Croatian translation of the Polymer Class Names document and it may be found at http://hrcaj.srce.hr/index.php?show=clanak&id_clanak_jezik=116145.

13.2. IUPAC-IUBMB nomenclature website

GM reported that there had not been a significant change in annual usage figures. The usage data were available at the website (<http://www.chem.qmul.ac.uk/iupac>) – at times there were 21 000 users per week, with atomic weights and the Periodic Table being the most popular.

13.3. IUPAC website

See minutes 6.(a), 6.(b), 9.7. and 12. for earlier discussions relating to the IUPAC website. In summary, what is needed is a website with improved visibility and usability, and where documents can be readily accessed. AY would be the contact person to facilitate this and he will be the conduit between the Division and Bryan Pearson or the Secretariat.

14. Reports from other IUPAC bodies

ICTNS – AY said there was little to report. He had received occasional documents and provided comment.

GM confirmed that there had been a lot of discussion in ICTNS around atomic weights and isotope work.

JCBN – GM reported that in the project on ‘Enzyme nomenclature and classification’, the list of enzymes was growing "exponentially". There were three relevant IUPAC projects, viz. ‘Nomenclature of flavonoids’, ‘Glossary of small molecules of biological interest’ and ‘Revision of carbohydrate nomenclature’. KHH reported that there were currently satellite meetings taking place.

CCE – Reference was made to the visit to the committee by the CCE delegation comprising its President, Mei-Hung Chiu, the Secretary, Jan Apotheker and an observer, Mary Garson, that had taken place the previous day. RMH described the various CCE meetings that were coming up in the next few days.

15. Any other business

15.1. International Standards Organization (ISO) liaison

The state of this liaison and the nascent projects had already been discussed the previous day and that discussion is reported above [*see minute 9.1.*]

15.2. Colour books e-mail consultancy

At the Division Committee meeting in Lisbon in July 2012 a proposal was made to have dedicated e-mail addresses to which the public could send comments and enquiries about the colour books. This correspondence would then at any time be directed to the person in charge of the colour book in question, but should at the same time be archived centrally so that the entire history could be displayed at any later time, even after changes in contact persons. After discussion, the present meeting decided that Bryan Pearson should be requested to install the e-mail addresses inorganic.nomenclature@iupac.org and organic.nomenclature@iupac.org. The address polymer.nomenclature@iupac.org already exists. AY proposed that a more general address, such as nomenclature@iupac.org, be used, with enquiries being redirected to the appropriate person. HR observed that there would be a need for clear work-flows and protocols. Indeed, there were dangers involved in opening feed-back channels and thought should be given as to how to moderate the flow of e-mails. It was agreed that AY would take care of this. Clearly discussions that took place earlier in the meeting are also relevant to this item [*see minutes 6.(b), 6.(e), 9.7., 10. and 13.3.*].

15.3. Other matters

15.3.1. Possible actions regarding Wikipedia

It was noted that Nigel Wheatley was involved in Wikipedia and might be able to provide some guidance. It was pointed out that whatever the Division did on Wikipedia could be changed by someone else! After some discussion no actions were proposed.

15.3.2. Discussion about Group 3 in the Periodic Table

This item arose from the 'Up for Discussion' article by Eric Scerri entitled 'Mendeleev's Periodic Table is finally completed and what to do about Group 3?' in *Chem. Int.* **34**(4), 28–31 (2012) (see <http://www.iupac.org/publications/ci/2012/3404/ud.html>). In his article Scerri presents an argument that he believes renders the newly proposed grouping of Sc, Y, Lu and Lr rather compelling, suggesting that any reluctance to accept this grouping as opposed to the more frequently seen grouping of Sc, Y, La and Ac for the Group 3 elements stems entirely from a reluctance to display the periodic table in a 32-column format. He furthermore proposes that IUPAC should take a stance on the membership of particular groups even if this has not been the practice up to this point. After some discussion it was clear that the committee was of the opinion that organization of the Periodic Table was not the business of the Division nor, indeed, of IUPAC.

15.3.3. Blue Book concerns

WHP asked the committee for advice on several matters raised in a letter from Janet Freshwater of RSC Publishing. Firstly, suggestions were invited for a design for the cover of the soon-to-be-published Blue Book (a suitable picture?); secondly, the exact shade of blue needed to be specified. The exact title of the book was then debated, and it was recommended that the title be changed to *Nomenclature of Organic Chemistry (IUPAC Recommendations and Preferred IUPAC Names 2013)*, i.e., move the year of publication to the end. It was also recommended that on the title page the private addresses of the authors be removed and replaced possibly with the IUPAC Secretariat's address. The committee further advised that Henri Favre's name should indicate that he was deceased, also giving the date of his death. Finally, KHH requested the committee to proofread carefully the lists of Commission and Division membership in the preface at the front of the Blue Book manuscript. [See also minute 8.2. for earlier Blue Book discussion.]

16. Dates and venue for next meeting

MB offered to host the Division Committee Meeting in 2014 in Bangor, Wales, UK, and this was accepted with the thanks of the Committee. MB warned that there was a long train trip from London to Bangor, of the order of 5 hours. The proposed timing would be in the last week of July to first week of August, possibly over the intervening weekend. The dates would need to be refined, depending on availability of University facilities.

It was also announced that the dates of the IUPAC General Assembly in 2015 would be 6–13 August, and that the venue in South Korea had been changed from Seoul to Busan.

AT THIS TIME, 10.50 AM, THE COMMITTEE DISPERSED TO TAKE PART IN THE CROSS-OVER MEETINGS REFERRED TO IN MINUTE 7.

[A summary of the proceedings at each of the cross-over meetings can be found in Appendix B.]

THE COMMITTEE RECONVENED AT 4.00 PM AFTER THE CROSS-OVER MEETINGS.

17. Adjournment

After a brief round-up of the cross-over meetings (see Appendix B), ATH offered a vote of thanks to the outgoing President of the Division, Richard Hartshorn, for his dynamic leadership over the last four years. As the Division's youngest President yet he had been inspirational and much had been accomplished in his

tenure. Based in the Antipodes, he may have been physically far removed from the rest of the world, but he was surely consistently close to the business of the Division, and he deserved the hearty congratulations and thanks of the Division. At the same time the Committee welcomed the incoming President for the next biennium, Karl-Heinz Hellwich, and wished him good luck and success in his tenure and offered him the full support of the Division.

The Division Committee meeting then adjourned at 4.30 pm.

Appendix A

(See minute 11.1.)

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

Appendix B

(See minute 7.)

Summary of feedback from inter-Division cross-over meetings

Divisions I and VIII

(Summary provided by ATH)

Division I was represented by Kaoru Yamanouchi (President), Anthony Goodwin (TM), Jürgen Stohner (TM and Chair of Commission on Physicochemical Symbols, Terminology, and Units), and Álvaro W. Mombrú (AM). Division VIII was represented by ATH, AY, and others.

Kaoru Yamanouchi gave an account of the main Division I activities, and AY and ATH described the current Division VIII projects. The idea of a project on the use of italic fonts was welcomed by Division I, and it was suggested that such a project would result in a Technical Report rather than a Recommendation, and that the conclusions would be a useful addition to the 'Green Book'. AY proposed that another useful project that might be of interest to Division I would be one on specifying how atoms should be numbered for spectroscopic and X-ray diffraction purposes. Possibly InChI could be used in some way as a basis for numbering atoms. This proposal was greeted with less enthusiasm, mainly because applications could not be seen other than for NMR spectroscopy. The Division I participants expressed an interest in nomenclature problems around energized (excited) molecules and moving hydrogen atoms, and this led to a discussion about Division VIII's nascent project on delocalization. The overall impression, however, was that there was not a lot of scope for joint projects at the present time.

Divisions II and VIII

(Summary provided by MB and ATH)

This meeting was chaired by the President of Division II, Bob Loss, with Lars Ohrström, Jan Reedijk and several other members of Division II present, while Division VIII was represented by MB, ATH, HR, EN and JR. The recent work of Division VIII was presented by MB (polyhedral boranes) and ATH (PINs, kappa grammar, central atom choice, flow chart of naming process, metallacycles), while HR made a PowerPoint presentation on InChI. Bob Loss was concerned that several projects initiated by Division VIII had slipped through the net as far as participation by or representation of Division II was concerned. After some discussion Daniel Rabinovich of Division II was nominated to join the new polyhedral borane and metallacycle task groups, while Sanjay Mathur was nominated to join the InChI task groups. Bob Loss confirmed that Division II would fund attendance of these nominees at the relevant task group meetings and that he would write to RMH in this regard. [*Secretary's remark*: Daniel Rabinovich attended subsequent meetings of the borane and metallacycle task groups on the following day.]

As far as the possible project in collaboration with ISO on metal clusters was concerned [*see minute 9.1*], EN would run the project proposal past Division II for possible membership and financial contribution.

Division II reported that Lars Ohrström's project on 'Coordination Polymers and Metal-Organic Frameworks' [*see minute 8.13*] had been completed, though there were still loose ends to be tied up in a future project focussing on nomenclature rather than terminology, and the expectation was that Division II would need to work with Division VIII on this.

Finally, mention was made of a possible new project from Division VIII to publish a revised version of the 'Red Book' in 2019, IUPAC's centenary year. The idea was received with acclaim.

Divisions III and VIII

(Summary provided by AR)

GM informed the meeting about the projects of Division VIII that might be of interest to Division III, namely:

- The 'Blue Book'
- The nomenclature of flavonoids
- Carbohydrate extensions and revision of the previous document
- 'Essentials' (brief guides to polymer nomenclature (already published), and inorganic and organic nomenclature (soon to be published))
- The project comparing four different systems for dealing with hydro prefixes (started at this meeting)
- The graphical representation of chemical reactions
- An area rather than a single project: InChI (International Chemical Identifier) that gives an alpha-numeric string representing the structure and you can go back from the string to the structure (unlike CAS)

Mary Garson presented Division III, and asked AR to describe the flavonoids project. She also requested that Division III be involved in the review process for the 'Essentials of Organic Chemistry', which was welcomed by KHH and GM. She informed the meeting about two projects that may be submitted:

- Nomenclature for metal-organic frameworks
- Nomenclature for bioconjugates

Concerning the latter project, AR noted that bioconjugates were presently named in the carbohydrate nomenclature project. GM confirmed that there are some compounds which are biologically active that have two units associated, which may be C-C linked, in which one is active and the other is not. This type of structure had not been named yet. KHH mentioned that terminology for biomedical materials and biodegradability, and bioterms for medicine, pharmacology, *etc.*, had been published by the Polymer Division and should be considered.

Mary also informed the meeting of the project already submitted by Mike Blackburn entitled 'Nomenclature of Transition States and their Analogs for Phosphoryl Transfer Reactions'. She also mentioned a possible project about the construction of a database to associate the structures of ligands with IUPAC names, both for phosphorus ligands and other types of ligands.

Mary then briefed the meeting on the 'Rules for Abbreviation of Protecting Groups', a Technical Report of Division III (Subcommittee on Organic Synthesis), and said that any other project on abbreviations will also be supported by Division III. It was mentioned that this document should be revisited for corrections.

KHH called for a revision of the class names of organic compounds and GM indicated that this project was concerned with terminology and Division III could certainly take this project for co-submission. Mary suggested circulating this project to see if any members were interested and she would get back to KHH with an answer. KHH said that the Division VIII budget could still take a project in this year, which could be on these class names, and Mary said that Division III had about 50% budget spent but she would check if a contribution were possible.

AY then explained that there had been a project on 'Glossary of Terms Used in Supramolecular Chemistry', which started 1995 and finished in 1999, from which nothing had appeared so far. Nobody knew who had been involved as chair or task group members. AY said that chemical topology could be the subject for a new project and that there were no recommendations, terminology or definitions concerning chemical

topology and supramolecular compounds, cage compounds, *etc.* He referred to the recent recommendations about rotaxanes and said that Division VIII would like to participate in a project on chemical topology, which could be joint between Divisions III and VIII, with task group members coming from both Divisions.

In conclusion, GM and Mary Garson commented how fruitful the meeting had been.

Divisions IV and VIII

(Summary provided by GM)

Very few members of either Division attended the meeting, which was also delayed from the original intended timing and was quite a short meeting.

Division VIII mentioned the almost completed revision of the Blue Book, which will assign preferred organic names. Other projects which were mentioned were the 'Essentials' summaries of both inorganic and organic nomenclatures, the 'Graphical Representation of Chemical Reactions' and 'InChI' projects– the latter especially with regard to its extension to polymers (presumably regular single strand polymers). Division IV expressed their concerns over source-based nomenclature, which required the use of traditional names – polyethylene, polypropylene, *etc.*, in contrast to the IUPAC names polyethene, polypropene, *etc.*

Appendix C

(See minute 8.8.)

Report on publications resulting from the project 2008-032-1-400, Basic Guidelines to Polymer Nomenclature

(Supplied by Roger Hiorns)

Original Article

A Brief Guide to Polymer Nomenclature, R. C. Hiorns, R. J. Boucher, R. Duhlev, K.-H. Hellwich, P. Hodge, A. D. Jenkins, R. G. Jones, J. Kahovec, G. Moad, C. K. Ober, D. W. Smith, R. F. T. Stepto, J.-P. Vairon, J. Vohlídal, *Pure and Applied Chemistry*, **2012**, 84(10), 2167-2169, DOI: 10.1351/PAC-REP-12-03-05

Reprints

A Brief Guide to Polymer Nomenclature, R. C. Hiorns, R. J. Boucher, R. Duhlev, K.-H. Hellwich, P. Hodge, A. D. Jenkins, R. G. Jones, J. Kahovec, G. Moad, C. K. Ober, D. W. Smith, R. F. T. Stepto, J.-P. Vairon, J. Vohlídal, *Chemistry International*, **2012**, November-December issue.

A Brief Guide to Polymer Nomenclature from IUPAC, R. C. Hiorns, R. J. Boucher, R. Duhlev, K.-H. Hellwich, P. Hodge, A. D. Jenkins, R. G. Jones, J. Kahovec, G. Moad, C. K. Ober, D. W. Smith, R. F. T. Stepto, J.-P. Vairon, J. Vohlídal, *Colloid and Polymer Science*, **2013**, January, 1-2, DOI 10.1007/s00396-013-2890-4

A Brief Guide to Polymer Nomenclature, R. C. Hiorns, R. J. Boucher, R. Duhlev, K.-H. Hellwich, P. Hodge, A. D. Jenkins, R. G. Jones, J. Kahovec, G. Moad, C. K. Ober, D. W. Smith, R. F. T. Stepto, J.-P. Vairon, J. Vohlídal, *European Polymer Journal*, **2013**, 73(1), iv-v, DOI: 10.1016/j.eurpolymj.2013.01.001

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A Brief Guide to Polymer Nomenclature, R. C. Hiorns, R. J. Boucher, R. Duhlev, K.-H. Hellwich, P. Hodge, A. D. Jenkins, R. G. Jones, J. Kahovec, G. Moad, C. K. Ober, D. W. Smith, R. F. T. Stepto, J.-P. Vairon, J. Vohlídal, *Polymers for Advanced Technologies*, **2013**, 24(1), i-ii, DOI: 10.1002/pat.3099

A Brief Guide to Polymer Nomenclature, R. C. Hiorns, R. J. Boucher, R. Duhlev, K.-H. Hellwich, P. Hodge, A. D. Jenkins, R. G. Jones, J. Kahovec, G. Moad, C. K. Ober, D. W. Smith, R. F. T. Stepto, J.-P. Vairon, J. Vohlídal, *Polymer International*, **2013**, 62(1), i-ii, DOI: 10.1002/pi.4442

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In Instructions to Authors

European Polymer Journal, Macromolecular Chemistry and Physics, Macromolecular Rapid Communications, Macromolecular Bioscience, Macromolecular Theory and Simulations, Macromolecular Materials and Engineering, Macromolecular Reaction Engineering, Macromolecules, Polymer, Polymer Chemistry, Polymer Degradation and Stability, Polymers for Advanced Technologies, Polymer Testing, Progress in Polymer Science, Reactive and Functional Polymers, Synthetic Metals ...

In Journal Editorials, Press and Society Pages

ACS Macro Letters Editorial, Chemistry International (and reprinted in its *purple paper version*), Macromolecules Editorial, MaterialsViews, Société Chimique de France