

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

**Minutes of Division Committee meeting  
Lund, Sweden, 12–13 August, 2010**

In attendance (the initials introduced here will be used throughout):

Richard Hartshorn (New Zealand), *President* **RMH**  
Gerard P. Moss (United Kingdom), *Past President*  
**GPM**  
Ture Damhus (Denmark), *Secretary* **TD**

***Titular members***

Kirill Degtyarenko (UK) **KD**  
Philip Hodge (UK) **PH**  
Alan T. Hutton (South Africa) **ATH**  
G. Jeffery Leigh (UK) **GJL**  
Jeffrey Wilson (USA) **JW**  
Andrey Yerin (Russia) **AY**

***Associate members***

Karl-Heinz Hellwich (Germany) **KHH**  
Jaroslav Kahovec (Czech Republic) **JK**  
Ebbe Nordlander (Sweden) **EN**  
József Nyitrai (Hungary) **JN**  
Warren H. Powell (USA) **WHP**  
Jan Reedijk (Netherlands) **JR**

***Observers and guests***

Michael J. Scott (USA) **MJS**  
Arthur Maximenko (Belarus) **AM**

The complete Division VIII Committee membership as of July 2010 is given in Appendix A.

**1. Introductory remarks and housekeeping announcements.**

Ebbe Nordlander and his staff were thanked for hosting the meeting.

**2. Apologies for absence.**

Jonathan Brecher (USA) and Hiroshi Ogino (Japan) had sent apologies beforehand. Amélia P. Rauter sent her apologies via KHH at the meeting. She had told KHH that she was not informed about the Division VIII meeting in Lund until they had contact shortly before.

[*Secretary's comments:* because of the suspicion that there might be problems of access to the web board, APR had been informed in a separate E-mail on 4 March, 2010, about the meeting dates in Lund. *APR had replied to this message.* However, in July, she had still – like others – had problems or apparent problems with access to the web board. The secretariat had checked that everything worked and APR was asked to return if problems continued. This was the last communication registered by the secretary from APR prior to the meeting.]

The total absence of national representatives was noted. The division recognises the problems of funding the participation of national representatives in Division meetings. A brief discussion ensued about using the internet facility Skype for enabling some kind of remote participation in meetings.

[The secretary understood that the committee wishes this to be brought forward again in connection with future meetings.]

**3. Introduction of attendees.**

A brief round of introductions was made around the table.

**4. Approval of agenda.**

The agenda was approved with remark that item 8.2 was moved to later in the day and that RMH wanted to give a brief report about the Division's finances just before embarking on item 9.1. Also, KHH said he would want to briefly mention a polymer project under item 8 that was not included in the agenda.

[*Secretary's note:* the finance report made by RMH has been minuted under item 14 below; the extra project mentioned by KHH is minuted as 8.8.9.]

## 5. Minutes of meeting in Glasgow, UK, 31 July–1 August 2009.

The minutes were approved with the proviso that the secretary implement the few remaining (trivial) corrections.

[*Secretary's note:* At the time of writing the minutes, the Glasgow minutes have been published on the IUPAC web site and on the Division web board.]

## 6. Matters arising.

With reference to Glasgow minute 13.4, KHH remarked that the decision made by the PAC editorial board to change the style of publication of technical reports and recommendations requires action because it does not ensure appreciation of all the contributions, in particular not major contributors of working-party members. If the publications are to parallel those of research publications, all contributors must be listed as authors. This is actually the way Chemical Abstracts have been handling IUPAC recommendations: All working-party members are listed as authors.

RMH said he would be willing to take this up in CPEP, but he would not be in a CPEP meeting before Puerto Rico. GPM said the solution is to list those persons as authors who actually contributed. PH said there are strong feelings in Division IV about authorship of such publications. JK remarked that not all task group members contribute to a given document publication process. AY mentioned that the rotaxanes document had only listed true authors. RMH and GPM stated that the task group leader must take the responsibility of ascertaining who contributed as authors. This means that it is important to clearly identify the task group leader. In any case, RMH promised to keep an eye on this matter.

## 7. Recommendations, translations and related publications since 2009 Division Committee meeting.

Bulgarian and Japanese translations of the Red Book 2005 were on GPM's web site.

GPM noted that there had not been Russian translations of nomenclature documents for a long while.

KHH made the following remarks concerning German translations of IUPAC Recommendations and Technical Reports:

The journal *Angewandte Chemie* since 2002 has been publishing translations of IUPAC Recommendations and Technical Reports into German. 28 translations were published from 2002 through 2007. After an interruption in 2008, two translations have been published in each of the years 2009 and 2010. Two of the translations deal with polymer terminology.

Of importance to Division VIII are the translations of the rotaxanes document in 2009 and the most recently published partial translation of the *Glossary of class names of polymers based on chemical structure and molecular architecture*:

**Karl-Heinz Hellwich, Elisabeth Weber:** Glossar von auf der chemischen Struktur und der Molekülarchitektur beruhenden Polymerklassennamen, *Angew. Chem.* 2010, **122** (28), 4943 – 4951 [original: *Pure Appl. Chem.* **81**, 1131 – 1186 (2009)]. [Translation only of excerpts.]

## 8. Division VIII projects.

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

Steve Heller's report from the InChI Subcommittee, dated 28 July, 2010, had been posted on the Division web board. The following list had been copied without further editing from the Division VIII project web page into the agenda:

Project No. 2009-042-1-800: InChI Requirements for Representation of Polymers

Project No. 2009-041-1-800: InChI Requirements for Representation of Markush Structures

Project No. 2008-035-1-800: IUPAC International Chemical Identifier (InChI) Symposium

Project No. 2008-033-1-800: InChI and InChIKey: Further Promotion

Project No. 2008-034-1-800: IUPAC International Chemical Identifier (InChI): Further Development

[*Secretary's note:* at the time of completing these minutes, two more projects in the same series had been approved and added to the Division VIII projects list:

Project No. 2009-043-2-800: Standard InChI-based Representation of Chemical Reactions

Project No. 2009-040-2-800: InChI Requirements for Representation of Organometallic and Coordination Compound Structures.]

Steve Heller not attending, AY first gave a summary of what the InChI is and a status on the development and use of it.

AY stressed that the InChI is not just a new SMILES string or another kind of 'Division VIII nomenclature'. The latter deals only with the naming of *drawn structures* [secretary's comment: not *entirely* true!], but InChI is able, to some extent, to code for *substances* as well. For example, there has been progress with respect to dealing with tautomers, and mixtures, such as needed by the polymer community.

In a world still lacking electronic representation standards, the InChI has been welcomed and is by now heavily used by database providers and regulatory bodies.

The IUPAC symposium project had been completed (the symposium having been held during the 2009 ACS Spring meeting). The 'Further promotion' project was also completed.

The 'Further Development' project deals with user requirements and was close to completion.

The weakest parts of the InChI at the moment were Markush structures and organometallics. In the latter area, there are many possible choices of structural representations to be used as input to the InChI program. Keith Taylor from accelrys participates in the organometallics project and had announced that a new molfile format was to be soon released.

AY concluded his introduction by stating that Division VIII should be very interested in the InChI and in promoting and controlling the development of it.

GPM mentioned that a large report is available on the standard InChI.

KHH said that new InChIs developed should be identical to older ones when applied to the same chemical entities, but AY said there will have to be changes, but also that conversion software will be available.

The reactions InChI project and the organometallics/coordination compounds InChI project had not been approved;

RMH said that after limited feedback from Division VIII, the secretariat was looking to find external reviewers.

Also, RMH and GPM mentioned that there had been insufficient detail in the original proposal for the reactions project.

[Secretary's note: as these projects are now approved and in the portfolio, as noted above, no more words will be spent on minuting that part of the discussion.]

TD cited Steve Heller's report, p.1, where it says: '...the Division VIII InChI Subcommittee oversees the development of InChI standards and is supported by IUPAC which approves them'. He asked what does it mean that 'IUPAC approves them'. InChI standards are very different from other IUPAC outputs.

It was eventually agreed that **TD** should contact Steve Heller and Alan McNaught after the Lund meeting to ask for an explanation and specifically to inquire about the role of ICTNS in relation to the InChI.

[Secretary's comments at the time of completing the minutes: extensive correspondence with, and shared by, Alan McNaught and RMH during the fall of 2010 made it clear that since 2004 it has been agreed that ICTNS cannot usefully contribute to reviewing output from the InChI project; and that IUPAC's involvement with the InChI project had been discussed in detail at the InChI Trust meeting in August 2010, at which a proposed description of that involvement had been put in writing and subsequently sent to RMH. The minutes of the following InChI Trust meeting (November 2010) mention that RMH had basically agreed to that description, taking only exception to a sentence indicating unreserved support from Division VIII to InChI Subcommittee members unable to cover their travel expenses. That particular sentence will be reworded. Otherwise, the description stated that ultimate responsibility for scientific requirements for InChI developments lies with the InChI Subcommittee; that the subcommittee would keep the Division VIII Committee fully informed of its activities and would welcome input from Division VIII; and that review of new InChI software version would continue to be carried out without the involvement of ICTNS, but by the subcommittee in consultation with a large number of actual users and administrators of chemical structure collections.]

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

WHP reported that the full draft of the IUPAC Nomenclature of Organic Chemistry in its new 2010 version was currently under review by the Division Committee and the Advisory Subcommittee, ostensibly for proofing and identifying inconsistencies. Unfortunately, a very large number of comments were being received, most of which (over 75 %) were the same comments that had been submitted for the 2004 draft. Comments on the 2004 draft, received from some 25 responders, had been thoroughly reviewed through correspondence and in multiday meetings of the Project Group (including Alan McNaught) in 2005 and 2007. (This can be verified by viewing the significant minutes of the Division Committee meetings in 2005–2007.) ICTNS had not yet reviewed the book and had recommended a further review due to the volume of comments appearing on the Division VIII web board, without knowing that most of the comments were repetitious and had already been thoroughly reviewed. The Division Committee suggested that each of the comments be reviewed again and a response to the reviewer provided for each comment. It was noted that the review of the 2004 draft was carried out in the same way as for the 2005 Red Book and all of the previously published reports by IUPAC and that no response to each comment was required. Hence, the procedure being suggested for the review of the New Blue Book was a radical departure from review procedures used in the past. WHP noted that this change in the review procedure would delay the production of the new Blue Book

significantly, perhaps by as much as two years. However, at the moment the procedure for review of the comments on the 2010 draft was that WHP drafted replies to all comments made on the web board, chapter by chapter, which were sent to HF. The consolidated replies from both authors were then posted on the web board.

WHP noted that the section on indicated and added hydrogen would be rewritten so as to make it clearer. He mentioned two issues for discussion:

(1) locants in conjunctive names (the IUPAC way vs. the CAS way);

(2) use of superscript locants for designating substituents on nitrogen characteristic groups. In 2007 CAS extended the use of such superscript locants in its index nomenclature.

These matters had also been discussed on the Division VIII web board.

(1) It was agreed to stick to the IUPAC placement of the locants in conjunctive names (*e.g.*, naphthalene-2-methanol). The suggestion was also made to abandon conjunctive names in the new Blue Book altogether. It was stated that conjunctive names as used in CAS index nomenclature was a nomenclature construction poorly understood by the community. WHP commented that there are a lot of nomenclature constructions that are poorly understood by the community. Anyhow, conjunctive names will not be used for PINs. RMH asked for opinions on keeping conjunctive nomenclature. A very few voiced an opinion. [*Secretary's remark*: after the meeting, it was considered that perhaps there had been doubt about the meaning of the question. So it would be appropriate to revisit the issue on the Division VIII web board.]

(2) It was decided to follow the use of superscripted locants for nitrogenous characteristic groups as used in CAS index nomenclature.

Other comments during the discussion included the following:

- AY mentioned the problem of nitrogen valence (do we want to use  $\lambda^5$ -N?).
- TD pointed out that the Blue Book in addition to providing preferred names will also be *the* new book of rules for organic nomenclature, including 'general nomenclature', so it will also be consulted by the educational system and this should be considered when writing it. WHP noted that there seemed to be a certain degree of misunderstanding about the purpose of the Blue Book. He recommended revisiting Alan McNaught's posting on the web board, explaining the original ideas behind the book.
- TD asked whether we can always use the principle of 'once blacklisted, forever blacklisted'. A good example is the names phosphine, arsine, *etc.*, explicitly designated as not acceptable any more in Red Book 2005. Can they reappear as acceptable in 'general' organic nomenclature in the Blue Book? No agreement was reached.
- Are the rules for constructing PINs in the Blue Book consistent? AY said his experience from testing the rules in his software was that they are "90 % consistent".
- WHP said it was not the intention to use footnotes in the new edition of the Blue Book.
- It was said that customers want names for substances, not for electronic structures, but another remark was that theoretical chemists may well want to have distinct names for *e.g.* distinct electronic structures.
- The draft contains clear markings of the places where rules have changed relative to earlier recommendations. However, it was also suggested to prepare a list of new structures named in the current draft.
- KHH mentioned the problem of the divalent substituent group names preferred in polymer nomenclature, but not in the Blue Book, *e.g.*, ethylene. (This aspect was discussed again under item 8.8.5 below.)
- As for the continued review process, **TD** promised to place the various chapters of the Blue Book in separate threads to ensure a clear separation of commentaries for them. He would also move the earlier comments to the relevant new threads.
- WHP asked that if one has non-trivial corrections, please propose a complete replacement text. WHP would then cut and paste as appropriate.
- AY was critical of the structural diagrams in the Blue Book draft. WHP said he could not draw structures at the moment because of software problems. ATH asked whether RSC would redraw the structures anyway.
- A project about collecting structural diagrams from the Blue Book was mentioned.

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

GPM had no progress to report.

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

GPM had no progress to report.

#### **8.5. Comparison of procedures for naming hydro derivatives of fused ring systems.**

This is not a project, but a draft document exists which also contains a treatment of mancude monocyclic system such as pyran. WHP noted that the material of the document is wholly contained in the new Blue Book. Nevertheless, GPM and KHH suggested completing the draft and publishing it separately. Bernardo Herold of ICTNS had made the same suggestion. WHP said there would be no time for this until after the Blue Book has been published. AY asked whether the draft could be posted on the web board. It was finally decided that **KHH**, **AY** and **AM** have a look at the draft together with **WHP** and consider preparing it for separate publication.

#### **8.6. Second edition of *Principles of Chemical Nomenclature, A Guide to IUPAC Recommendations* (2006-029-1-800).**

GJL reported that ICTNS had received (although with some delay due to computer problems at their end) the entire manuscript for review with a deadline of 16 September, 2010. However, *Principles* would not be submitted to RSC on 16 September. GPM said it should be published in any case before the Puerto Rico 2011 meeting. KHH asked about the price of the book. ATH suggested producing a softback version but GPM replied that this is almost as expensive as a hard-cover book.

TD commented upon the editorial review of the book and stressed the importance of the new *Principles* being in complete agreement with the latest Red Book and the upcoming Blue Book. Could one envisage hiring a person to do dedicated editorial review like we have done with the Blue Book.

During the meeting, GPM posted the latest version of the book on the Division VIII web board for further commenting from the Division VIII Committee and Advisory Subcommittee members.

[Secretary's note: the production plan for *Principles* was revisited under item 9.5 below.]

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

RMH reported from the project group meeting held the day before, where several Division Committee members had joined as observers. There had been good discussions, and good progress had been made; this encourages us to also arrange for synergy with the Division Committee meetings in the future. The document on extensions of the kappa convention was close to being ready for submission as a recommendation. Selection of central atoms was the next subject to be dealt with.

Financially, the funds for the project were exhausted, but once there is output, one might look at asking for an extension of the project.

#### **8.8. Polymer projects (with Division IV).**

[Secretary's note: items 8.8.7 and 8.8.9 deal with projects that are formally not shared between the divisions.]

##### **8.8.1. Source-Based Nomenclature of Single-Strand Organic Polymers (2003-042-1-800).**

KHH told that the project is nearing completion. During the last year, more or less minor editorial work has been done. The task group met during the last meeting of the Division IV Subcommittee on Polymer Terminology in Glasgow in July this year with a few points raised there. Tatsuki Kitayama had asked KHH to present the revised draft he prepared after the discussions in Glasgow. In order to allow Division VIII members a non-influenced look at the document, KHH had distributed the document on 26 July, 2010, and later also posted it on the Division VIII web board. Tatsuki and the working party seek feedback from Division VIII and a general expression of Division VIII opinion on the major content of the document and of course general approval before going into final editing before the usual approval procedure.

For source-based names, of course the currently preferred names for monomers are recommended. Polymer chemists need a set of retained names for very frequently used compounds (*e.g.*, adipic acid, caprolactam).

In 2007, Tatsuki presented an earlier draft of this document to the Division VIII Committee (Turin minute 9.5.2). At that time GPM asked Tatsuki to provide a list of retained names that Division IV regards as important. This is now done with this draft.

Specific points on which clarification and approval is required:

- are the retained names listed acceptable?

- should trivial or retained names for polymers be given first or the systematic names?
- is it essential to define a specific order of monomers in source-based names of copolymers, *e.g.* alphabetical order. The question of the order of name components for copolymers was raised by GPM last year.
- Is it acceptable to define retained (trivial names) for polymers not declared as source-based (or structure-based) names? Actually this is already done for polyethylene! These names would then be acceptable or in some cases even preferred names besides the usual systematic source-based or structure-based names.

Following the discussion, it was agreed that Division members should look again at the document and comment on the web board within 4 weeks.

#### **8.8.2. Nomenclature for Chemically Modified Polymers (1999-051-1-800).**

PH told that the project had been thoroughly discussed in Glasgow, and external reviewers were now being sought (a slow process, however). PH considered the project to be interdivisional. RMH suggested **posting the draft** on the Advisory Subcommittee web board.

#### **8.8.3. Nomenclature for Rotaxane Polymers (2007-009-1-800).**

AY addressed this project. J. Vohlidal is the chairman. The paper has been through public review. It is in agreement with the discrete rotaxanes document.

#### **8.8.4. Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers (2001-081-1-800).**

JK told that the document is still in preparation. It was originally a nomenclature document, but now some TG members think it must contain more terminology as well. JK remarked that it is a very specialized subject, even for polymer chemists. KHH said there had been long discussions about this project in Glasgow in July 2010 during the meeting of the Division IV Subcommittee on Polymer Terminology, and good progress had been made. JK said the document had been split in two, but it was now being considered to unite them again. Alain Fradet has undertaken the task to prepare this draft. Jiri Vohlidal, JK, Werner Mormann, Alain Fradet and KHH are going to meet by the end of this year in order to prepare a final version.

KHH and GPM made remarks to the point that the nomenclature required in this document should be provided by Division VIII. **JK** said he would have the latest version of the dendrimer part and the necessary basic terminology posted on the Division VIII web board.

#### **8.8.5. Preferred Names for Polymers – a list of preferred, acceptable (other IUPAC-approved) and not acceptable (wrong or outdated) names for polymers (2008-015-1-400).**

There had been little progress in this project. After the meeting of the task group leader, Werner Mormann, and KHH in Glasgow on 2 August 2009, it was clear that the provided beta version of the database program intended for the systematic extraction of names for polymers and constitutional units of macromolecules from IUPAC documents needed some improvements. Unfortunately, the programmer did not respond. So, it was decided in April 2010 to do the work without the program. Mormann and KHH selected two IUPAC documents out of which they wanted to prepare a table as a sample. This should then be used by the members of the working party for the work on all other IUPAC documents. The sample tables up to now contain some twenty entries.

KHH mentioned the well-known problem with names of divalent substituent groups appearing in polymer backbones. Irrespective of the Blue Book preferred substituent group prefixes, the polymer community may insist on ethylene, the reason being that all groups outside the polymer backbone are treated as substituents, leading to 1-methylethylene rather than propane-2,1-diyl, *etc.*, which makes ethylene the most common group name in structure-based polymer names at all.

There seemed to be agreement around the table that a few such well-entrenched exceptions, for use in backbone naming *only*, would be acceptable.

A draft document is hoped for at the end of the year.

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

PH said the guide in question is only for the web. It was anticipated that the project would start serious work in a year's time.

#### **8.8.7. A brief guide to polymer nomenclature (polymers 'essentials') (2008-032-1-400).**

The chairman is Roger Hiorns. The title of the document was now *Brief Guide to Polymer Nomenclature*. It was to be a two-page overview, intended for publication not only in *Pure and Applied Chemistry* but also in all journals in the polymer area – so to speak as an addition to their author guidelines. In addition, it was envisaged to distribute it as a card, similar to the 4-page Green Book condensate handed out at the IUPAC General Assembly in Turin in 2007.

During the meeting of the Subcommittee on Polymer Terminology (SPT), 6–9 July in Glasgow, the TG met together with some observers. At this meeting a well-advanced draft was thoroughly revised, which resulted in a draft in which probably only minor adjustments would be necessary. This draft had been circulated to the working party together with some specific questions. Comments were expected before 30 September 2010. After performing necessary corrections, a professionally paginated draft copy of the document was to be prepared which would then be sent to journal editors and managers for their comments and modifications.

After that, the working party would discuss comments and make necessary changes. This meant that the project was nearing completion and approval by SPT could be expected in 2011.

KHH circulated a recent version of the two-pager at the meeting.

[Secretary's note: this project is listed as a project solely for Division IV on the IUPAC web site.]

#### **8.8.8. Definitions and Notations Relating to Stereochemical Aspects in Polymer Science (2009-047-1-400).**

KHH told that the TG had a constituting meeting during the meeting of the Division IV Subcommittee on Polymer Terminology on 8 July, 2010, in Glasgow. All but one member were present.

In principle, the project is a revision of the document *Stereochemical Definitions and Notations Relating to Polymers* published in *Pure Appl. Chem.* **53**, 733–752 (1981) and reprinted as Chapter 2 in the Purple Book and (with minor editing) as Chapter 2 in Purple Book 2.

A brainstorming resulted in a number of potential and/or necessary actions during the revision of the existing document on stereochemical description of polymers. Most importantly, the section on the use of *meso* and *racemo* needs a revision because the terms are widely used in polymer sciences but the usage in polymer sciences is contradictory to the usage in organic chemistry.

The discussion resulted in a preliminary scope of the project which was agreed upon, according to which the project will start with a revision of the 1980 recommendations with a primary focus on the basics necessary to describe stereochemical aspects of polymers. Special problems which are less important and cannot be resolved quickly should be left out and considered for a follow-up project (in order to avoid a too large project which will never finish). The addition of a section on the description of absolute configuration is essential. The section *Specific terminology for crystalline polymers* should be removed (keeping a few paragraphs moved to other sections). On preparing the draft the view should be into the future, in order to prepare a document providing recommendations which will (still) be valuable in about 10 years.

The announcement of the project had been published in *Chem. Int.* **32**(4), 20–21 (2010). Online version and PDF are accessible via [www.iupac.org](http://www.iupac.org) under the *Publications* tab.

#### **8.8.9. Guidelines for abbreviating polymer names (2006-004-1-400).**

This Division IV project was nearing completion. KHH said it is of interest to Division VIII because it will include an extended list of currently used abbreviations for names of polymers. One major task during the final stages of this project will be to create IUPAC names for all the entries in the table because this table will include a large number of abbreviations based on non-IUPAC names. Many of these abbreviations are taken from the ISO list and the ASTM list.

#### **8.9. Nomenclature of Flavonoids (2009-018-2-800).**

Amélia P. Rauter not being present, KHH told that this project had been approved but had not really started yet. Because of the volcano activity in April, the meeting scheduled to take place along with the JCBN meeting in Cambridge could not take place. Amélia Rauter was working on the preparation of a draft for discussion in a future meeting. However, date and place of this meeting had not yet been decided upon (except that Portugal had been suggested).

## 8.10. Other interdivisional projects.

### 8.10.1. Classification, terminology and nomenclature of borophosphates (2003-034-1-200).

[Project with Division II]. The project is completed. JR mailed the final report to RMH and TD during the meeting. However, the same information is displayed on the IUPAC web site under the project number 2003-034-1-200.

### 8.10.2. Recommendations for nomenclature and databases for biochemical thermodynamics (2006-023-3-100).

The bottom line was that the project was still in a deadlock. Originally a JCBN project, it became a formal Division I project, but is, in reality, a project between IUPAC and IUBMB. There was some discussion about such inter-union projects in general and about the activities of IUBMB-NC, but no specific actions.

### 8.10.3. Coordination polymers and metal organic frameworks: nomenclature guidelines (2009-012-1).

[L. Öhrström is the chairman; JR is in the project group; this is formally a Division II project]. The group is working. In addition to nomenclature guidelines, it is necessary to deal with terminology.

See the description of the project in *Chemistry International* **32** (1), 23 (2010).

JR's report is included as Appendix B. There may be a final report to present already in Puerto Rico.

[Secretary's note: see also remarks about projects on inorganic and coordination polymers under item 9.6 below.]

## 9. Future projects/activities.

### 9.1. Graphical representation of reactions (W.G. Town?).

### 9.2. Graphical representation of polymers (JK, KHH).

Both projects can be viewed as split out from the original graphical representation projects. There was no news from Bill Town on either. According to KHH, the polymers project is not currently on the agenda of the Division IV Subcommittee on Polymer Terminology. However, it has been noted that information and guidelines on graphical representation of polymers are scattered over several documents. Moreover, the 1994 document on graphical representation of polymers is not completely consistent with the recently published document on Graphical Representation Standards for Chemical Structure Diagrams.

The need for having a drawing software package to work with polymers was discussed, and it was noted that project funds could be used to cover that expense.

RMH agreed to contact Bill Town about both projects.

### 9.3. Metallacycles (ATH, WHP).

ATH noted that this project is on hold while the inorganic PINs project discusses problems of how to select and order central atoms.

### 9.4. Boron nomenclature.

GJL would contact Michael Beckett about getting involved with this subject.

### 9.5. Division VIII activities in the International Year of Chemistry 2011.

It was discussed whether the launch of *Principles* should be in some way coordinated with other 2011 activities, or staged at Puerto Rico, or whether it would be better to distribute activities over the entire year.

GJL was to contact RSC about the timing for publication of *Principles*.

KHH mentioned the eventual preparation and printing of 'essentials', concise guides to the various areas of nomenclature similar to the 4-page Green Book condensate handed out at the IUPAC General Assembly in Turin in 2007. The polymer 'essentials' had been already dealt with under item 8.8.7. It was discussed whether the nomenclature essentials should be 2, 4 or 6 pages (6 pages would be a 'fold out' concept).

RMH volunteered to draft an inorganic essentials and KHH an organic one. The drafts would be posted on the Advisory Subcommittee web board. The question was put whether the latter draft should be based on the 1993 rules or the rules of the current Blue Book draft.



## 9.6. Other projects.

Metal clusters are relevant to the contact to ISO regarding nomenclature/terminology in the nanoparticle area (cf. item 14.3). There had been no scoping exercise for metal clusters (yet).

AY needed experts for a project on rotaxane stereochemistry. He was not going to activate the project during 2010, however. The project will be mentioned under future projects in 2011.

Recommendations for naming delocalised systems. TD reminded about the problem of how to name ligands of the acetylacetonate type. Preferred names for coordination compounds containing such ligands will of course require preferred names for the ligands. TD reminded that it had been promised in Büdingen (2008 meeting, minute 8.2.3) that the Blue Book would provide rules for this, but TD did not find such rules. WHP said Henri Favre had taken out the discussion of such delocalized systems. It was agreed that a group must get together to discuss how to proceed in general with the naming of delocalised systems. **JK**, **AY**, **ATH**, **TD** agreed to participate in this exercise, and **KHH** said he was interested to be kept informed. A project proposal could perhaps be worked out already in 2010. **TD** volunteered to initiate these activities.

The Division IV Subcommittee on Polymer Terminology (SPT) had the intention to submit a project proposal regarding nomenclature for inorganic polymers at the initiative of Dick Jones. Current guidelines are from 1985. This project would explicitly exclude coordination polymers. It would be intended to provide an update for the part of the material for which expertise is available within SPT. It was asked whether anybody in Division VIII would be willing to join the task group or knew of persons interested. [JR during the meeting E-mailed three names of potential task group members to JK. **JR** and **JK** to decide on further action.]

In this context it was also asked could anybody imagine participating in a separate project on coordination polymers or do we know of interested persons? Could members of the task group under 8.10.3 be recruited for this?

## 10. Membership.

### 10.1. Status of Division VIII Committee membership.

Current membership, see Appendix A.

### 10.2 Elections for the biennium 2012-13.

Various rules and practicalities around the elections and some still moot points were mentioned by RMH and GPM and discussed.

Some important points were:

The Division needs new blood and everybody was encouraged to think about this. Importantly, anybody can get involved by assuming task group leadership and will obviously then be welcomed as an observer at Division Committee meetings. This is one possible way into the system.

Present members who wished to continue in one of the membership categories in the Division Committee should consider that there is a time limit for titular membership for which membership of Division Committees count, but not former membership of Commissions. Only AY was eligible for continued titular membership. There are possibilities for waivers so that individuals may be prolonged beyond that time limit. Everybody should check the lists sent out to see if their history of membership in IUPAC bodies and thus their eligibility for the various officer posts and membership categories were correctly given there.

National representatives have to be nominated by their NAO.

In any case, RMH is continuing as president, but there was to be an election for vice president. Only current titular members can stand for vice president. The electorate for the VP election is the Division Committee.

The Bureau must see the lists of TMs at the meeting in April 2011.

**RMH** was to communicate via the board regarding the elections and **TD** to help checking the membership.

[*Secretary's note:* Since the Lund meeting, GPM became chair of the Nominating Committee and asked for nominations in a message posted on the Division and Advisory Subcommittee web boards on 27 September 2010.]

### 10.3 Advisory Subcommittee.

Current membership, see Appendix A. Again, the first action was for **RMH** and **TD** to check out the current members – *i.e.*, is the list up to date. A message could be put on the web board urging current members to consider proposals for new members.

## **11. Division discussion board. Still not an ideal tool?**

[*Secretary's note while minuting:* the object of this item tends to be called by various names, including 'web board' and 'discussion board' and constructions involving the term 'forum'. The title of this item has been kept for historical reasons, but otherwise, for consistency, 'web board' is used throughout these minutes (KHH's contributed notes in Appendix C have not been reworded, though). There are two web boards relevant in the present context, with different readerships, one for the Division Committee and one for the Division Advisory Subcommittee. They may be collectively termed 'the web board'.]

Whereas the web board has acknowledged advantages in terms of enabling the sharing of large files, KHH was mostly critical of this facility and mentioned his reasons. These were sent in written form to the secretary and are included here in Appendix C. Some division members had had problems accessing the web board or receiving alerts from it, probably (partly) because of local firewalls at the receiver end. As a result of the discussion, **TD** suggested he invite Bryan Pearson from the IUPAC secretariat to the next meeting in Puerto Rico to discuss functionality of the web board. In the meantime, it was agreed that it would be a good idea to always write in a web board message what material was posted along with it, and perhaps also to send out an E-mail to relevant recipients to make sure those persons became aware that the posting was made.

## **12. Publicity.**

### **12.1. IUPAC and IUBMB nomenclature web site.**

GMP reported that the web page continued as usual and as usual there were seasonal variations in the frequency of use of the site. Thus, changes were expected again after New Year.

### **12.2. IUPAC web site.**

KHH said the new IUPAC homepage certainly has some advantages but it has definitely a large number of disadvantages. Most importantly, the web site is bad publicity – the old homepage no longer being updated, the new one not working properly and missing important information.

**TD** mentioned that it is not easy to find one's way to the 2004 Blue Book draft on the web site and that the naming service is also deeply buried. In addition, the naming service does not always provide names that are in accord with existing recommendations. (**TD** had had some correspondence with **AY** about this based on an inquiry sent by a user who got a name according to the 2004 rules, not the 1993 Blue Guide rules. **AY** said it would be difficult to be completely consistent in this period where software is being developed towards the expected new Blue Book rules. And in fact, the naming software on the web is some 5 years old by now.)

Nobody seemed to disagree with the criticisms of the web site. **RMH** promised to keep the subject alive at meetings higher up in the IUPAC system.

### **12.3. Other publicity issues.**

Nothing to minute.

## **13. Reports from other bodies.**

### **13.1. Committee on Chemistry Education (CCE).**

**RMH** reported. The main activity in CCE is the planning of the Chemical Education conferences. There had only been short working group reports at the latest committee meeting. **RMH** had told about the upcoming publication of *Principles* (cf. items 8.6 and 9.5 above) in 2011.

### **13.2. Committee on Printed and Electronic Publications (CPEP).**

No report had been received. **TD** was instructed to inquire whether a report is available, and to be also proactive in requesting one well in advance of next year's meeting.

### **13.3. Committee on Chemistry and Industry (COCI).**

No report had been received. **TD** was instructed to inquire whether a report is available, and to be also proactive in requesting one well in advance of next year's meeting.

### **13.4. PAC editorial board.**

A report from the latest meeting was included already in the 2009 Glasgow minutes, cf. item 6 above.

### 13.5. Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS).

GPM mentioned that there had been a meeting for titular members. No report was presented.

In connection with ICTNS's areas of responsibility, KHH remarked that an update and supplement of the guidelines on the use of italic and roman fonts might be helpful. **JK**, **GPM**, **TD**, and perhaps **KHH** expressed an interest in working with this, and **GPM** promised to take an initiative.

### 13.6. Report from 2010 JCBN meeting.

GPM told that the annual JCBN meeting had been hit by the volcanic ash problems. The meeting had taken place in Cambridge, but with limited attendance. There had been no meeting on the small molecules project, which was still awaiting a reply from Dick Cammack in connection with the approval process in the Project Committee.

The Enzyme Nomenclature group was busy; currently 20-50 new enzymes were added to the list per month.

[*Secretary's remarks:* The membership for JCBN listed in Appendix A was taken from the Division VIII homepage just before the Lund meeting and is still the same there in January 2011. The secretary notes that the project list for JCBN at this time is empty, *i.e.* presumably not updated.]

## 14. Any other business.

### 14.0. Finances.

On the morning of the second day, RMH provided a status of the Division's finances.

[*Secretary's comment:* this was not on the agenda; we should perhaps make it a regular agenda item in the future?]

With a total budget for the current biennium of USD 80,000, Division VIII had a somewhat larger budget than the other divisions. As of 3 August 2010, the status was as follows:

Committed (for projects):	USD 19,700 (24.6 %)
Operational expenditure:	USD 21,183 (26.5 %)
Funds remaining	USD 39,117 (48.9 %)

Thus, at this point in the biennium, the Division had spent just over half of the budget. The guideline for project commitment for the biennium is USD 56,000, while that for operations is USD 24,000.

Further project commitments were expected soon, as several projects were in the final stages of review.

Spending a large fraction of the guideline operational expenditure is expected as the off-year divisional meeting is the major operational expense for the division. Generally speaking, Division VIII tends to spend more than the guideline on operational activities, not the least because scoping studies and other project development activities fall into this category of expenditure. So far this biennium, some InChI activities, and attendance at an IUPAC-ACS liaison meeting and an ISO meeting had been funded from operational expenditure.

### 14.1. Proposal re the periodic table by P.G. Nelson (posted on Division web board 26 May, 2009).

GJL had written a letter to Prof. Nelson that had been approved by RMH and TD. However, GJL told that in fact many correspondents are worried about the periodic table. Some say teachers do not like the IUPAC table and that it is largely ignored.

GJL had suggested to Prof. Nelson to approach CCE, but Nelson's thinking was that Division VIII must take responsibility for the table.

GJL said he was happy to set up some kind of investigation to get some hard evidence on the community's views on the periodic table and use of the IUPAC layout. As a specific action, **GJL** agreed to talk to JR as new vice-president of Division II. Also, **ATH** and **TD** promised to probe the school systems in their own countries regarding attitudes toward particularly the IUPAC layout of the periodic table. **GJL** himself would get in touch with the Association for Science Education in the UK (see <http://www.ase.org.uk>). Contributions from other countries would be more than welcome and should be sent to GJL.

EN said 2011 would give opportunities to distribute again a printed version of the periodic table. GPM said what happens on the web is more important, and KD remarked that everybody consults the webelements site (<http://www.webelements.com>) about matters relating to the periodic table and the elements.

#### **14.2. Input for ICSU strategic plan for 2012-2017.**

Excerpt from 28 June, 2010, letter from IUPAC Executive Director Terry Renner to the Divisions:

The Secretariat has received a request from ICSU to provide information to assist them with the preparation of their Strategic Plan 2012-2017. The attached document describes what is needed from us. There are three items related to energy that need a response. The Secretariat will take care of Item 1. Your specific comments regarding Item 2 are most important and these don't need to be long or detailed. Please feel free to comment on any of the three Items if you wish.

The document in question had been posted on the Division VIII web board together with the agenda draft. The request from the secretariat for input from the division was discussed. **TD** was instructed to reply to the secretariat to the effect that we consider there is little overlap with the work going on in Division VIII.

#### **14.3. Meeting of ISO/TC 229 (Nanotechnology) in Maastricht, 18 May, 2010.**

RMH reported. ISO has a Technical Committee (TC229) dealing with nanomaterials [including gold clusters, carbon nanotubes, and entities yet to be defined (and discovered)] and is considering nomenclature and terminology in that area (and thinking about the differences between the two concepts, which may not be as sharply separated there as we are used to). They had approached Division VIII to explore possibilities for a collaboration. Currently this was also being considered at upper levels of the two organisations. (JCBN is an example of a body bridging IUPAC and another similar international organisation and has existed for decades.) ISO works very differently from IUPAC, however; there are very complex voting and consensus procedures, *etc.*

RMH had had a number of contacts with ISO TC 229 representatives via E-mail and telephone conferences, and on 18 May, there had been a meeting in Maastricht, the Netherlands, which TD attended physically while RMH was partially on-line. The next meeting was to be in Kuala Lumpur and would be attended by RMH.

There were no specific actions at the time, but eventually RMH might be looking for potential task group members.....

#### **14.4. Renewed contact with Andreas Dress.**

**TD** would send a reply to Dress expressing our interest in renewed contact (could be in connection with item 14.3) and suggesting Division VIII get in touch as soon as we feel ready to re-explore the collaboration with AD.

#### **14.5. Other issues.**

KHH asked what had happened to the 'apprentices' arrangement set up in Glasgow – should the names of the apprentices be published? It was decided to first have an internal round. **RMH** and **TD** would start by getting in touch with the apprentices via E-mail.

#### **15. Date and time of next meeting in Puerto Rico.**

Information at the time of the meeting pointed to the General Assembly being held from 30 July through 4 August, Council being on 3–4 August. Most probably, the Division VIII Committee meeting would be on 30–31 July.

#### **16. Adjourned.**

## Appendix A. Memberships.

### Division VIII Committee, membership as of 12 July, 2010 (as listed on the IUPAC website)

Richard M. Hartshorn (New Zealand)

*President*

Ture Damhus (Denmark)

*Secretary*

Gerard P. Moss (United Kingdom)

*Past President*

*Titular Members*

Jonathan Brecher (United States)

Kirill Degtyarenko (United Kingdom)

Philip Hodge (United Kingdom)

Alan T. Hutton (South Africa)

G. Jeffery Leigh (United Kingdom)

Jeffrey Wilson (United States)

Andrey Yerin (Russia)

*Associate Members*

Karl-Heinz Hellwich (Germany)

Jaroslav Kahovec (Czech Republic)

Ebbe Nordlander (Sweden)

József Nyitrai (Hungary)

Warren H. Powell (United States)

Jan Reedijk (Netherlands)

*National Representatives*

Ricardo Bicca de Alencastro (Brazil)

Sundarababu Baskaran (India)

M. Abdul Jalil Miah (Bangladesh)

Patrick Moyna (Uruguay)

Hiroshi Ogino (Japan)

Rolando F. Pellón (Cuba)

Amélia Pilar Rauter (Portugal)

### Subcommittee on the IUPAC International Chemical Identifier (membership as copied directly from the Division VIII webpage on 5 August, 2010)

*Chair*

Heller, Stephen R.

*Secretary*

McNaught, Alan D.

*Members*

Bachrach, Steven M.

Batchelor, Colin

Bolton, Evan

Goncharoff, Nicko

Goodman, Jonathan M.

Nicklaus, Marc

Pletnev, Igor

Rey, Hinnerk

Stein, Stephen E.

Steinbeck, Christoph

Taylor, Keith T.

Tchekhovskoi, Dmitrii

Williams, Antony

Yerin, Andrey

**Division VIII Advisory Subcommittee**

(membership as copied directly from the Division VIII webpage on 5 August, 2010):

Abe, Hidetsugu	Katritzky, Alan R.
Bachrach, Steven M.	Laitinen, Risto S.
Brennan, John	Mata, Paulina
Bünzli-Trepp, Ursula	McCann, Graham F.
Campagnari, Ilaria	Pabel, Jörg
Carter, Jeffrey P.	Pecoraro, Vincent L.
Connelly, Neil G.	Poulter, C. Dale
Cooke, Helen	Schepers, Hervé
Cozzi, Franco	Scott, Michael J.
Degtyarenko, Kirill	Sloan, Thomas E.
Donovan-Merkert, Bernadette T.	Smith, Ann
Dress, Andreas	Stein, Stephen E.
Fairhurst, Geoffrey	Taylor, Keith T.
Favre, Henri A.	Thilgen, Carlo
Gibney, Danièle J.	Thomas, Sarah
Giles, Patton M.	Thurlow, Kevin
Godly, Edward W.	Town, William G.
Goodman, Jonathan M.	Traynham, James G.
Gottlieb, Harry	Wilks, Edward S.
Herold, Bernardo Jerosch	Wisniewski, Janusz L.
Ihlenfeldt, Wolf-Dietrich	Yuan, Shen-Gang
Jenkins, Aubrey D.	

**IUBMB-IUPAC Joint Commission on Biochemical Nomenclature (JCBN)**

(membership as copied directly from the Division VIII webpage on 5 August, 2010):

*Chair*

Schomburg, Dietmar

*Secretary*

Cammack, Richard

*Members*

Moss, Gerard P.

Tipton, Keith F.

Vliegenthart, J. F. G.

*Associate members*

Cornish-Bowden, Athel

Horton, Derek

## Appendix B.

### Report for Division VIII on the project in item 8.10.3.

(JR on behalf of Lars Öhrström, 12 August, 2010)

#### **Coordination polymers and metal organic frameworks: terminology and nomenclature guidelines.**

MOF-project Division II, with Division VIII. Chair: Lars Öhrström, Gothenburg.

The project started 1 August 2009.

The objectives of this project are (1) to produce guidelines for terminology (glossary of terms) and nomenclature (concerning topology, not naming of individual substances) in the area of coordination polymers, (2) to ensure that these guidelines are accepted by a large group of leading researchers in the field, and (3) to have these guidelines implemented or referred to in the instructions to authors of leading general and inorganic chemistry journals.

Activities:

1. Meeting in Glasgow;
2. E-mail exchanges between project team members.
3. Article in: *Chem. International* (January 2010).
4. Working documents going around.
5. Collecting definitions from textbooks and review works.
6. Questionnaire in preparation for 2 leading journals (*Cryst. Eng. Commun. Crystal Growth and Design*).
7. Lectures at Conferences by team members: addressing the project (like ICCG, Adelaide, 2010; Pacificchem, 2010).
8. Meetings (ad hoc; not IUPAC supported) by team members in subgroups.

Our inaugural meeting in Glasgow served to highlight some of these differences, but also to clarify the origin of these different practices. It was also very useful exercise creating a good working ambiance in the group. Following this we have had frank discussions over the IUPAC web board with these 4 main points:

1. The creation of a questionnaire to be sent out to the editorial boards of leading journals in the field. This will use web technology based on Google documents and a few test runs have already been made.
2. A proposition from the chairman for the definition of MOF and a subdivision(classification) has been discussed.
3. It has emerged that sole use of "coordination polymer" is a term not acceptable by many scientists from the solid state field.
4. As "coordination polymer" is already sanctioned by IUPAC for 1D chain polymers it has been proposed that "coordination polymer" could be used as the general term for any 1D, 2D or 3D system, but that for the 2D and 3D systems the term "coordination network solid" could be used to further characterize a compound. In this way the term coordination polymer can be retained, but providing an IUPAC alternative to those who are opposed to this term. This has been accepted by many of group members, but not yet by all, thus discussions are still in progress.

## Appendix C.

### Notes by KHH regarding the Division VIII web board (see item 11).

When discussing about the discussion board, there are certainly a number of points to be raised – some of them maybe in comparison with the old web-board and with yahoo groups.

- As compared with a standard way of communication, namely e-mail, the web-board is not user-friendly.
- The web-board certainly has some advantages but it has definitely disadvantages.
- It is not obvious who the recipients are of what I put onto the web-board.
- A posting cannot be copied (*e.g.* as a proof of action) to somebody else (as I did with the source-based document, when I copied Tatsuki Kitayama).
- The alert e-mail messages I receive from the web board do not contain any specific subject information in the header. I must open them in order to know what they refer to. [They all are listed as “New post/Thread information: ... (Please do not reply ...)”]
- Similarly, the messages I receive from the web board do not contain any specific sender information. I must open them in order to know who posted a message. (They are all listed as from IUPAC Discussion board.)
- Hence an automatic categorising of messages in the e-mail program by sender or subject is not possible (they all go into a folder web-board which is more or less like a dust bin showing hundreds of messages with the same sender and subject).
- The additional login to a separate platform is not user-friendly and makes me use it only in rare cases, *i.e.* if absolutely necessary (up to last week only for downloading files).
- The structure of the web-board is not very clear.
  - There are postings in the thread Messages from the President which are posted by others.
  - Replies are not marked as replies.
  - I cannot post a second message under the same heading unless I classify it as a reply (*e.g.* my thread Lund meeting – my second posting was not a reply to myself. Similarly, under the heading Messages from the President I would not expect any reply).
  - A thread marked as moved is still accessible from the list, while it is not indicated why and where it is moved.
  - There are threads in the Archive to which contributions for discussion are still posted.
- Uploading a file is more or less a lottery. You cannot see where it goes before you upload the complete posting.
- Users added to a forum, obviously do not get access information (I received a request from Jörg Pabel several weeks ago stating that he did not know how to access the web-board [I could help him]. And Amélia Rauter wrote that she was not informed about the Lund meeting. Actually this was done completely via the web-board).
- Unfortunately, since last Saturday (just after my last posting) I could not login again. I always was returned back to the login page.
- Direct answer to a posting out of the e-mail programme would be desirable.
- The web board should not use cookies and java script.
- Automatic logout (*i.e.* a timeout) must not be too short (not less than 1 h).