Ture Damhus/June 2014
These minutes were approved in Istanbul 2013 but only submitted after the final JCBN 2012 minutes could be inserted as Appendix D in June 2014

International Union of Pure and Applied Chemistry
Division VIII
Chemical Nomenclature and Structure Representation
Minutes of
Division Committee meeting
Lisbon, 2-3 July, 2012

1. Welcome, introductory remarks and housekeeping announcements.

2. Attendance.
Present: Richard Hartshorn (President; RMH), Karl-Heinz Hellwich (Vice President; KHH), Ture Damhus (Secretary; TD), Michael Beckett (MB), Ebbe Nordlander (EN), Warren Powell (WHP), Hinnerk Rey (HR), Andrey Yerin (AY), Philip Hodge (PH), Jeff Wilson (JW).
Observers: Bernardo Herold (BH), Arthur Maximenko (AM), post-doc Nuno Manuel Xavier (Faculty of Sciences, Lisbon).

Apologies: Md. Abul Hashem, Alan Hutton, Antony Williams, Jonathan Brecher, Gerry Moss, Gernot Eller, Jaroslav Kahovec, Kirill Degtyarenko, Jan Reedijk.
Amélia Rauter had been responsible for arranging all the practical details for the meetings in Lisbon, but had had to cancel her own participation because of a meeting in Brussels regarding funding for her academic projects.

No message received: Nigel Wheatley, Wei Huang, József Nagy, Sundarababu Baskaran, Itrat Anis, Lupituko Luko Mkayula, Supawan Tantayanon, Vefa Ahsen.

3. Introduction of attendees.

4. Approval of agenda.
Items might have to be switched around. Otherwise no comments.

5. Approval of minutes of meeting in San Juan, Puerto Rico, 28-29 July, 2011.
The latest draft (dated June 20) had been circulated via E-mail on June 20. The minutes were approved. Note, however, comments under item 6 below.

6. Matters arising.
In relation to San Juan minute 9.2, WHP expressed the Blue Book authors' unhappiness about the many comments that came in repeatedly during the review process as if those submitting them thought they could force through late changes in this way; the authors considered this kind of correspondence to be a slight on their professionalism.
It was agreed that RMH contact Fabienne Meyers about the still pending obituary for J. Nyitrai.
EN brought up the problem of funding for National Representatives (NRs) to go to Division Committee meetings with specific reference to the situation of Md. Abul Hashem, whom he had personally interacted with. Hashem could not attend due to lack of funding. RMH said that the Division budget *could*, in principle, be used for such a purpose, but that it would be better to involve NRs in projects. Several attendees pointed to the possibility of having web meetings. RMH replied that one could consider having some Division

members participate on-line at the General Assemblies, where facilities for this could perhaps be placed at our disposal more easily than at off-year meeting facilities.
With reference to San Juan minutes 7 and 15.4, it was agreed that TD should contact Alan Hutton and Jan Reedijk to learn whether there had been any further activities within the Interdivisional Subcommittee on Materials Chemistry.
With reference to San Juan minute 9.2, KHH noted that in fact 'acetylamino' is recommended in the carbohydrates document.
There had been issues with the Division VIII discussion forums. Due to the uncertainties regarding, *e.g.*, whether members are prompted when there are new postings, and the fact that the Secretariat was into a busy period and would not be likely to be able to help fast, it was decided to carry out all correspondence, circulation of documents, *etc.*, via E-mail for the time being.

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

RMH said we have to engage with SPT (the Division IV Subcommittee on Polymer Terminology) on a regular basis. One way is to work at having joint members. KHH pointed out that SPT does not follow the 2-year cycle the rest of IUPAC is subject to. But in any case we can send observers to each other's meetings.
KHH said that historically, there had been nomenclaturists from the former Macromolecular Commission in SPT, but now SPT is looking for more polymer nomenclature experts.
PH also reminded that there *are* true joint projects. RMH said perhaps there should be a special project number for joint projects. Joint projects (with joint sponsoring) are encouraged within IUPAC. RMH would inquire with Fabienne Meyers (who assigns project numbers) about this.
In any case, the discussion ended with the conclusion that RMH should talk to the Division IV officers about the situation and in particular discuss closer collaboration between the Divisions and with SPT.
It was also suggested that ICTNS should be contacted to make sure they always involve Division VIII in any document dealing with nomenclature.

8. Updates on Division VIII projects.

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

AY, HR, and Anthony Williams are involved in InChI projects.
AY and HR gave a general introduction to InChIs via examples shown on a few slides. HR pointed out that whereas standardisation of traditional nomenclature aims at improving communications between humans, what InChIs do is basically to facilitate communication between machines.
The polymers InChI project had been completed; other projects were in progress.
AY pointed out that InChIs may be helpful in situations where there are multiple representations of structures.
In that context, RMH mentioned that the recent project on tautomer representations (Proposal #2012-023-1 entitled "Redesign of Handling of Tautomerism for InChI V2", to be coordinated by Marc Nicklaus) had been recently approved. DivisionVIII was to supply half of the funding and the Project Committee presumably the rest. Apparently not all Division VIII members had been able to view the April 29 posting on the web board regarding this project proposal or had not been prompted via E-mail to have a look. (See more about the web board elsewhere.) RMH reported that the external referees had been very positive about the proposal. AY explained that InChI handling of tautomerism until now had been rather of an 'experimental' nature.
AY said there are several channels through which IUPAC could provide more funding for InChI work. The idea was aired that the InChI Subcommittee could be merged with CPEP. There was also interest in having more interaction with industry and more general reaching out to the chemical community. This, however, should probably be handled in the InChI Trust (in which IUPAC is represented by the Executive Director).
RMH said that we should think strategically about InChI projects when manning Division VIII. KHH suggested that we attempt to have the InChI Subcommittee meet adjacent to Division VIII meetings for better communication, although it was well understood that there are other restraints on those meetings.

RMH brought up the question whether InChIs or InChIKeys could conceivably be associated with barcodes. Barcoding takes place in many of the settings where InChIs are foreseen to be of value (chemicals registration *etc.*). TD strongly supported investigating this aspect.
At the end, HR mentioned that he was preparing to draft a proposal for a project to deal specifically with inorganic InChIs and urged anyone interested in participating to let him know.

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

WHP summarised the history of the project briefly as follows. It started at the initiative of Henri Favre as the *preferred-names project* already during the period when the 1993 Blue Guide was under preparation for publication. WHP became significantly involved from 1998. The first draft of the resulting 'new Blue Book' was presented for comment in 2004, and the comments received were considered by WHP, HF and Alan McNaught during 2006–2007. A revised draft was ready in 2010. Again comments were received and considered for the final revision. HF and WHP were of the opinion that many of these comments did not warrant further discussion. Others were clearly swayed by the number of comments and paid little, if any, attention to the quality of comments. A quick analysis of some 300 comments on P-65 by Ursula Bünzli-Trepp quickly revealed only some 20 comments that led to substantial changes in text, a rather small percentage.
In San Juan in 2011, the editing of 7 out of the 10 chapters with respect to the comments received had been completed, and the last three had now been edited, including comments about the naming of isotopically substituted compounds made by Jonathan Brecher.
The Royal Society of Chemistry had asked for the information they need for publicising the book and were prepared for publication in 2013. The publication of the book will be enabled by using a camera-ready manuscript of the entire book prepared by WHP. This manuscript was almost complete even now; the main remaining (and ongoing) task was to go carefully through Appendix 2, a 50-odd pages list of prefixes to be used in substitutive nomenclature, ensuring that the prefixes in this list were actually introduced in the main text with their status (preferred or otherwise) assigned to them. Issues about seniority of classes in Chapter 4 brought up recently by AY were to be addressed, as far as possible. It was still under consideration how to generally best summarise or highlight the changes made relative to the current recommendations.
According to previously agreed-upon plans, the completion of the book by HF/WHP was to be followed by an editorial review, *i.e.*, an independent person should go through the text and check cross-references, spelling errors, consistency, *etc.* (the exact extent of this review was still to be decided). Marcus Ennis of EBI had expressed interest in taking on this task and was expected to end his current employment so as to be available from mid-August.
KHH and TD expressed concern that if the version now available went directly via this review to the publisher, Division VIII would be endorsing the book after a process in which many comments had been only briefly replied to with a "no", and in which the Division had not seen the text since 2010. However, WHP was hesitant to share the camera-ready version because he was concerned that further discussions might arise that could imply changes with wide-ranging consequences for *e.g.* pagination and cross-references, and he expressed that he was not prepared to undertake any further editing at this time.
It was decided after some discussion that as soon as WHP had completed the above-mentioned last editing tasks – which might be even before Marcus Ennis initiated his review – the entire book should be made available for inspection by the Division Committee. RMH was to work with Fabienne Meyers about how to enable the large-file transfers involved.
It was reminded that in principle, ICTNS must also review the final version. However, BH said he assumed that ICTNS would be satisfied with a very quick review process in view of the fact that the basic review had taken place in 2005. The process now would be that the book went via RMH to ICTNS, and RMH would provide a cover letter with appropriate explanations about the development of the book and its current final status.

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

KHH reported from Gerry Moss that there was no progress. BH said he remembered the ICTNS review of the document: objections from reviewers were easily overcome, so what is the problem? TD was charged with asking Gerry Moss what his perspective was and whether the Division could somehow help progressing it.

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

Similar discusion as item 8.3. The document was initiated by the late Hal Dixon. TD will inquire about this project as well.

8.5. Comparison of procedures for naming hydro derivatives of mancude ring systems.

Nothing had happened since the latest draft of the document had been circulated following the San Juan meeting. BH commented that the document could become a valuable technical report. AM volunteered to work on the document so as to finalise it before the end of the year as a technical report for publication in PAC.

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

The book had been published and brought to the closing ceremony of the International Year of Chemistry in Brussels in December 2011.
KHH reported about the indexing process. He had still discovered numerous errors while indexing. Furthermore, the printed version had not been identical to the last file he had forwarded. TD expressed the hope that similar things would not happen with the Blue Book.
KHH would circulate the RSC advertisement for the book.

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

RMH reported that the task group was currently worrying about particular problems in connection with the applications of the kappa convention. He expressed the hope that the kappa document could soon be published, and that the group could work in parallel on the choice of central atoms. In the end, one should maybe consider making a long list of PINs.

8.8. Basic Guidelines to the Nomenclature of Organic and Inorganic Chemistry ('Essentials' of organic and inorganic nomenclature) (2010-055-1-800).

The chairmanship was shared between RMH and KHH. RMH presented the status of the documents. It was agreed that preferably, the published guidelines should be both available at the Istanbul General Assembly. An ordinary review process should not be necessary, since the documents do not contain new recommendations.

8.9. Polymer projects (with Division IV).

Note: **Below, 'SPT' will consistently denote Division IV's *Subcommittee on Polymer Terminology*.**
KHH had participated in the recent SPT meeting in the USA (Roanoke, VA, June 2012) and did most of the reporting under item 8.9.

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

KHH summarised the long discussion at the SPT meeting that had followed our Division VIII Committee meeting in San Juan in 2011, mentioned the developments since then and reported from the Roanoke meeting. Four very different drafts of the document had been produced since San Juan. The title of the document had changed in the meantime to 'Source-Based and Traditional Nomenclature for Homopolymers, Copolymers and Graft Polymers'. The main

issue, polymer names based on monomer names no longer acceptable according to IUPAC recommendations, had been finally settled by introducing the polymer names in question as *retained polymer names*. KHH hoped that a short and *limiting* list of such names could be finally agreed on. About 20 polymers for that list had been mentioned in Roanoke.

8.9.2. Nomenclature and Graphical Representations for Chemically Modified Polymers (1999-051-1-800/2006-006-1-800).
KHH discussed the document sent out via E-mail on 28 June, 2012. This project was considered complete by the task group except for a few minor issues that needed clarification. The plan was to have a 1-month period for review by both Division VIII and SPT, after which the document could hopefully be submitted to ICTNS.

8.9.3. Nomenclature for Rotaxane Polymers (2007-009-1-800).
This project was discussed several times during the Division Committee meeting. At first it seemed that Division VIII had not been informed about the latest draft of the document, even though it is formally a 800 project, but in fact it had been posted on the Division VIII web board on September 12, 2011, with a 1 month deadline for comments. In the meantime, public review had been completed, but AY noted that the comments received had only recently been circulated in the task group. In any case, the document was in the proof phase, and a very short deadline was now needed if anyone would have more comments.
[*Secretary's remark:* the minutes are kept brief here in view of the fact that at the time of writing them, the rotaxane polymers document has been published: Terminology and nomenclature for macromolecular rotaxanes and pseudorotaxanes, *Pure Appl. Chem.* **84**(10) 2135–2165(2012); doi: 10.1351/PAC-REC-11-10-15.]

8.9.4. Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers (2001-081-1-800).
The working party had met in Roanoke, but the document was not yet ready for review.
[NB: This item may need elaboration.]

8.9.5. 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).
Since the 2011 meeting, almost all IUPAC polymer documents had been screened for names of constitutional units (CUs). These were extracted and collected in several tables (Excel xls files). Since some working party members did not break the units down to simple CUs without subunits, some additional editorial work had to still be done before the tables could be merged and screened for duplicate entries. After completion of this work a final classification of all names for CUs as preferred, acceptable and not acceptable was to take place.

8.9.6. 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)
In the absence of the task group leader (PH), Dick Jones had chaired a task group meeting at the SPT meeting in Roanoke; most of the SPT members had been present. A draft prepared by PH a few weeks before the meeting had been discussed, first concerning questions and annotations by PH and then page by page, where only page 5 had been reached. Nevertheless, the general view was that only minor points remained to be resolved, most of them concerning standardisation of fonts and formatting.
The revised draft prepared during this meeting as well as comments by KHH not dealt with in Roanoke were to be returned to PH for preparing a new draft to be distributed later in the fall to the working party for comments.

8.9.7. A brief guide to polymer nomenclature (polymers 'Essentials') (2008-032-1-400).
There had been discussions in Roanoke about the not optimal review processes between SPT and Division VIII in the year following the San Juan meetings. A number of comments made by TD and KHH and Jaroslav Kahovec had been discussed at Roanoke. The ferrocene example would stay but the complete section has been revised and was now suitable. The formulae were all to be redrawn. Three young observers, all working in the area of materials chemistry/optoelectronic polymers, had been present and had contributed positively to the work on the document.
[*Secretary's remark:* at the time of writing these minutes, the document has been published: *Pure Appl. Chem.* **84**(10) 2167 – 2169 (2012), and was included as a two-page tear-out in *Chemistry International* **34** (6)(2012).]

8.9.8. Definitions and Notations Relating to Stereochemical Aspects in Polymer Science (2009-047-1-400).
In Roanoke, the task group, jointly chaired by KHH and Graeme Moad, had discussed various details of their document: the use of rotated Fischer projections, the terms constitution, configuration and conformation as defined in "Basic Terminology of Stereochemistry" and the terms constitutional repeating unit, configurational unit, configurational base unit and configurational repeating unit in the document. Different definitions for some of the terms in several documents needed to be considered. A number of actions had been agreed upon.

8.9.9. Guidelines for abbreviating polymer names (2006-004-1-400).
After the 2011 SPT meeting, a new draft had been prepared and distributed for comments. During the 2012 meeting in Roanoke, the task group had dealt with these comments and a revision of the document based on these comments. Again, a general discussion on the principal organisation of the document had arisen. However, the main conclusion had been that the manuscript was close to completion. A new draft based on the discussions in Roanoke was expected to be prepared by the task group leader, Jiasong He, by August 2012. Working party approval and SPT approval were expected by the end of the year so that the document could then be sent for public and ICTNS reviews. The major remaining task, owned by KHH, was to check or provide all the IUPAC names for the extended list of abbreviations in the appendix. For this, some information on the meaning of the abbreviations and the names currently given in the table was still needed from other SPT members.

8.10. Nomenclature of flavonoids (2009-018-2-800).
BH reported from the project on behalf of Amélia Rauter, the task group leader. The task group had met in Hinxton, UK, in May in connection with the JCBN meeting (cf. item 14 below).The group had worked at defining various classes of flavonoids. Regarding nomenclature, there was a desire to express preference for particular names, but the term 'preferred name' could not be used.

8.11. Other interdivisional projects.

8.11.1. Recommendations for nomenclature and databases for biochemical thermodynamics (2006-023-3-100).
The document had been published [*Biophys. Chem.* **155** (2011) 89–203.]

8.11.2. Coordination polymers and metal-organic frameworks: nomenclature guidelines (2009-012-2-200).
TD to inquire with the task group leader, Lars Öhrström, about the status of this project. [*Secretary's remark:* the document, which was basically a terminology document, was subsequently forwarded to RMH and other Division members for commenting – leading to the removal of *names* that could not yet be assigned on the basis of existing IUPAC nomenclature recommendations – and at the time of writing the minutes, it has been sent on in the system and is up for public review until April 2013.]

8.11.3. Terminology and Nomenclature of Inorganic and Coordination Polymers (2011-035-1-800); for short TINCOPS.
KHH reported that the project (in which TD participates as a task group member) had been discussed at the Roanoke meeting. The objective of the project is the long overdue revision of the 1984 document 'Nomenclature for Regular Single-Strand and Quasi-Single-Strand Inorganic and Coordination Polymers'. The project is funded in equal measures by Divisions II, IV and VIII. The document being worked at included relevant terminology as well as nomenclature. The Roanoke meeting had discussed a preliminary listing of terms requiring definition along with relevant polymer class names, prepared by Dick Jones, the task group leader. TGMs were to supply structures that would exemplify the naming principles that should be covered in the nomenclature sections.
A young observer who had shown interest in the project, Michael Walter, had been welcomed as a new task group member.

8.11.4. Glossary of small molecules of biological interest (2009-022-2-800).
KHH and TD reported from the meeting of the task group in Hinxton, UK, in May 2012, in conjunction with the JCBN meeting (cf. item 14 below). There are thousands of 'small molecules', and the project has a problem in keeping the list of entries at a manageable length. TD pointed out that the document is not a glossary; PH said often a concise database of this kind is considered to be a glossary. HR pointed out that many existing databases containing similar information are not of good quality. He would be able to supply material from other databases that might be relevant for the project.
There was some concern that the Division is the official sponsor of the project, which is joint between IUPAC and IUBMB, but does not really know what it is about. RMH agreed to take contact with the task group chair, Dick Cammack, to get a better understanding of the goals of the project.

8.11.5. Abbreviations for protecting groups (2011-044-1-300**).**
RMH and Amélia Rauter are task group members; the leader is Margaret Brimble. BH mentioned an earlier incarnation of the project that had been discontinued after intervention from ICTNS. HR issued a warning not to make distinctions between abbreviations dependent on the use of upper or lower case letters. The document was to be discussed soon after the Division VIII meeting.

9. Future projects/activities.

9.1. Graphical representation of reactions (2003-0045-3-800).

The original project on graphical representation standards was completed by the publication of the two recommendations on structural diagrams and stereochemical configuration (referenced on the IUPAC web site). RMH mentioned that due to the very efficient organisation of the project, not the least thanks to Jonathan Brecher, there was still money available that could be used for the new extension to chemical reactions. Bill Town (who was not present) had gathered the new task group which had met the day before

the Division Committee meeting. RMH said that if the project used up the remaining money, they could apply for an extension.
TD said there is terminology involved that the group must define carefully and with a view to what is already in the Gold Book.
KHH reminded about the late Don Nicholson's metabolic pathways maps (now available form Sigma-Aldrich), also a graphical representation of reactions, and it was suggested to mention them to Bill Town.

9.2. Graphical representation of polymers.

KHH reported that there was basically no news. There are bits in existing documents that need to be taken into consideration.

9.3. Metallacycles.

EN said that there was no news to report, but he mentioned the existence of the old metallacycles document and agreed to prepare (with Alan Hutton) a proposal for a project to work on that document before next year's meeting in Istanbul.

9.4. Boron nomenclature.

MB went through a report he had sent recently to the President with a status on boron nomenclature. The report is included here as Appendix C.
The Committee endorsed the idea of reworking the boron chapter in the Red Book. MB agreed to undertake the drafting of a project proposal. AY (and later TD) expressed interest in teaming up for this.

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

The Division considers the completion of Principles (item 8.6 above) and the initiation of the Essentials for inorganic and organic nomenclature (item 8.8 above) to be the main activities in 2011 that complied with the overall vision and goals of the IYC.

9.6. Other projects.

Rotaxane stereochemistry.
AY said the project needs to address terminology problems in the rotaxane area. He reported that he had worked hard at recruiting task group members but with no success. The reply was always a polite refusal. He had considered extending the project to cover catenanes as well. Various potential contacts were mentioned. TD promised to ask Prof. Stefan Vogel, University of Southern Denmark, whether he might be interested. There should be possibilities with colleagues working in the general field of chemical topology.

Delocalised systems.
TD had not had time to initiate the scoping exercise that had been discussed in San Juan. HR advised to see whether there were suggestions for approaches to delocalised systems to be found in the InChI projects.

Crown nomenclature.
PH pointed out that it is not useful to keep on naming crown ethers as such. KHH said that systematically, they should be named as heterocycles, perhaps in some cases as fused rings systems. He did not see an urgent need for a specialised document, however.

Nomenclature terminology.
There are terms (like 'suffix', 'ending', 'substituent', 'trivial name', 'semisystematic name') that are needed in the exposition of IUPAC nomenclature rules, but which are not defined or are inconsistently defined. Hence the suggestion that the Division consider some kind of project on such terminology. There was not unanimous enthusiasm for this, however. EN suggested to put such work

'on the backburner'. RMH said one could let the terminology we recommend disseminate 'parasitically' in textbooks, *etc*. In conclusion, no action for the time being.

A central web page for finding all IUPAC recommendations/publications.
It was agreed that it would be useful to have a better overview of all IUPAC nomenclature recommendations on the IUPAC website. A good alternative at the moment is Gerry Moss' website at http://www.chem.qmul.ac.uk/iupac. In spite of the need, it was not considered a real project issue, but rather something to be discussed with the Secretariat. HR pointed out that it would be good to work at improving the Wikipedia page about IUPAC. (See also items 13.3 and 15.4 below.)

Document on *italic* and roman fonts. It was pointed out that this issue is really of an interdivisional nature. BH pointed out that ICTNS does not have projects in the ordinary sense. KHH said he would contact the ICTNS chairman about ways to address the subject.

– In addition, there was discussion under this item of new proposed project themes (catenanes, knots, chemical topology, tetrapyrroles, calixarenes). This was basically a brief brainstorming and no decisions were made.
It was suggested that in looking for new Division Committee members in the future, it be considered that they should bring in expertise on some of these areas.

10. IUPAC expert nomenclaturists: suggestion forwarded by Alexander Senning.

The proposal as presented in Appendix B (which had also been attached to the draft agenda) was discussed. There was some uncertainty as to who would be the potential users, what about payment, and it was mentioned that experts also make mistakes, so what about liability/insurance. RMH said there were good thoughts behind the proposal; perhaps it should be more a consultancy than a direct naming service. In any case, TD was charged with bouncing the case back to Senning and urging him to elaborate the proposal further with more focus on the pros and cons.

11. Membership.

11.1. Status of Division VIII Committee membership.

For the 2012-13 roster, see Appendix A.
The process for elections for the 2014-2015 biennium had already begun. Division VIII has a somewhat wider electorate than other Divisions. RMH explained about the criteria for choosing titular members: we have to consider subject expertise, geographical distribution and opportunities for organisational interactions within IUPAC. But the Division always welcomes observers; their funding could typically be secured via involvement in a task group.

11.2. Division VIII representatives in other IUPAC bodies, in particular ICTNS and JCBN.

AY had replaced Jeff Leigh in ICTNS.
RMH was currently associate member of CCE.
RMH was also on the PAC board which only meets at the general assemblies. He encouraged anybody interested in stepping in to indicate this interest.
As for JCBN, Gerry Moss was now the chairman and TD and KHH were associate members.
See also item 14 below.

11.3. The Division VIII Advisory Subcommittee.

The current roster probably needs updating but there was no specific action.

12. Division web board with discussion forums.

Several attendees mentioned problems with the web board, whether when trying to upload or download documents or not receiving prompts when new postings were made. Apparently the organisation

(FIZChemie) maintaining the web site until recently was to stop and the immediate perspective for remedying the deficiencies was not clear.
The Secretary was to contact the Secretariat about the problems.

13. Publicity.

13.1. Recommendations, translations and related publications.

Recent Japanese translations were mentioned (the *Red Book* and another Japanese nomenclature book, a kind of guide book covering inorganic, organic and polymer nomenclatures).
A Russian group was at work translating the *Blue Book*. RMH to contact that group to emphasise that a new edition of the Book was on its way.
BH told about the work going on with translations of the *Red Book* into Portuguese as well as Brazilian Portuguese. He was also trying to make a case for having *Principles* (cf. item 8.6 above) translated into Portuguese.

13.2. IUPAC-IUBMB nomenclature web site.

No particular news.

13.3. IUPAC web site.

See also items 9.6 and 12 above.
A discussion took place on the current appearance and function of the new IUPAC home page. The impression was that it had been rushed onto the web. Some liked the way it looked, others thought the design was non-intuitive, but there was general dissatisfaction with the functionality: the search engine did not work properly, the project lists were not updated, the structure is also non-intuitive. It was agreed that the Secretary should collect further comments until July 15.
[*Secretary's remark:* this deadline was eventually extended a few days, but only one or two further comments were received. Communication with the Secretariat in subsequent months was put on hold because of obvious resource problems at the Secretariat, and although a message has later been sent regarding the problems with the project lists, no significant progress is in sight at the time of writing these minutes.]

13.4. Other publicity issues.

It was discussed whether it would be worthwhile issuing a Division VIII newsletter. EN thought not. TD said small news items might be of interest, but it was also mentioned that the Division ought to make more use of *Chemistry International*. RMH agreed to this as far as to give 'diffuse encouragement'.

14. Reports from other bodies.

AY, the Division VIII representative, had no news to report from ICTNS. He had not been able to participate in the recent (Spring 2012) meeting, and had not been prompted to review any documents. KHH said that he had been notified of several documents for review via his NAO. AY promised to check once again that all necessary communication channels to ICTNS were open.
[*Secretary's remark*: the other two ICTNS members from Division VIII, Gerry Moss and Amélia Rauter, were absent with apologies.
The minutes from the ICTNS 2012 meeting are available in the meantime on the IUPAC web site.]

TD and KHH reported from the meeting of JCBN in Hinxton, UK, in May 2012. Both had been elected associate members of JCBN. KHH briefly mentioned ongoing JCBN activities regarding carbohydrate nomenclature and bioinformatics. One detail of interest was that it had been discussed whether 'Essentials' in the current Division VIII sense of the term should be produced for biochemical nomenclature or parts thereof.
[*Secretary's remark June 2014*: The JCBN 2012 minutes are included here as Appendix D after final approval at the 2014 JCBN meeting.]

RMH reported from the Bureau that Mark Cesa was working at his Vice President's Critical Assessment. He would be emphasising preparations for the IUPAC centenary in 2019 and would be having a strong focus on IUPAC connections to outside organisations.
There were already bids for hosting the IUPAC general assemblies in 2017 and 2019.

KHH mentioned that at the SPT meeting in Roanoke, he had given the presentation on the Blue Book that he also gave in Brussels in November 2011 (cf. item 15.3 below). It had been well received, in particular with the young observers present.

RMH mentioned that the CCE was to meet in July, so no news before then.

15. Any other business.

15.1. International Standards Organisation (ISO) liaison.

The last meeting RMH had attended in this context was in mid-June 2012 (ISO TC 229 at ISPRA in Italy; he had notified Division VIII via the web board on June 1 and invited further attendees). ISO have identified the most relevant materials to work at first as being metal clusters, metal oxides, carbon nanotubes, various core-shell structures and noncrystalline materials such as cellulose.
In the context of clusters, TD promised to send EN the old document by Coucouvanis.
Mention was made of Chris Ober's project *Terminology of Nanomaterials and Nanotechnology in Polymer Science* (2012-001-1-400) and RMH promised to take contact to Ober.

BH mentioned that Anders Thor, ISO TC 12 representative to ICTNS, had passed away in the spring. He asked about future ISO membership of ICTNS; ICTNS itself do not think they should necessarily again have a representative from ISO TC12.

15.2. Colour Books E-mail consultancy.

The idea was to have dedicated E-mail addresses to which the public could send comments and inquiries 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 when contact persons had maybe changed. KHH mentioned that the soon to be published Polymers Brief Guide (cf. item 8.9.7 above) was to include such an E-mail address. In the preface to *Principles* (cf. item 8.6 above), the IUPAC Secretariat E-mail address was given as the place to direct comments.
KHH had discussed the idea and the technical aspects with Bryan Pearson at the IUPAC Secretariat shortly before the DC meeting. It was agreed to wait and see if Bryan would eventually be able to set up a system for the colour books before investigating other possibilities.

15.3. Workshop on chemical names and their translation in Brussels, November 2011.

A draft article about the workshop by RMH and the Brussels organiser Hervé Schepers (from the European Commission's Directorate-General Taxation and Customs Union) was with Fabienne Meyers and was to appear in *Chemistry International*. TD said the workshop had been useful, but it was a pity that the presentations and other material had still not been posted on the internet as promised.
[*Secretary's remark:* the article later appeared in *CI* **34** #6 (2012) 29–32.]

15.4. Other matters.

Possible actions regarding Wikipedia were discussed, and project 2011-013-2-400: *Updating Wikipedia: Synchronizing Polymer Definitions and Terminology* was noted.
KHH said he had bad experiences with changing material posted in Wikipedia. Material could be changed again soon afterwards, so was it worth bothering? Anyway, the above project had started, and perhaps the general way

forward would be to post not editable text, but 'images' that could not be changed.

Of other matters, RMH summarised the Division's budgetary situation. According to IUPAC guidelines, most of the spending (≈ 70 %) should go to project work and the lesser part to divisional operations. Historically, the Division has typically spent more that 30% on operations, principally because of commitments to support InChI activities and engaging with other organisations such as ISO. Titular members should be actively engaged in projects. It is important that we maintain a high level of project activity and this will lead to full use of the Division budget allocation.

16. Date and venue for next meeting.

The exact dates for the Istanbul meetings were not yet available, and the Division needed an overview of which task group meetings were to take place in conjunction with the DC meeting. The Secretary was to take care of this.

17. Adjournment.

The meeting was adjourned in the early afternoon of July 3.

Appendix A

Division VIII, final roster for the biennium 2012-13

Prof. Richard M. Hartshorn (TM-President 2010-2013) New Zealand
Dr. Ture Damhus (TM-Secretary 2012-2015) Denmark
Dr. Karl-Heinz Hellwich (TM-Vice President 2012-2013) Germany

Dr. Michael A. Beckett (TM 2012-2013) United Kingdom
Prof. Ebbe Nordlander (TM 2012-2013) Sweden
Dr. Warren H. Powell (TM 2012-2013) United States
Prof. Amélia Pilar Rauter (TM 2012-2013) Portugal
Dr. Hinnerk Rey (TM 2012-2013) Germany
Dr. Antony Williams (TM 2012-2013) United States
Dr. Andrey Yerin (TM 2010-2013) Russia

Dr. Kirill Degtyarenko (AM 2012-2013) Spain
Prof. Philip Hodge (AM 2012-2013) United Kingdom
Prof. Alan T. Hutton (AM 2012-2013) South Africa
Prof. Jan Reedijk (AM 2012-2013) Netherlands
Dr. Nigel Wheatley (AM 2012-2013) United Kingdom
Dr. Jeffrey Wilson (AM 2012-2013) United States

Prof. Md. Abul Hashem (NR 2012-2013) Bangladesh
Prof. Wei Huang (NR 2012-2013) China/Beijing
Prof. József Nagy (NR 2012-2013) Hungary
Prof. Sundarababu Baskaran (NR 2012-2013) India
Prof. Itrat Anis (NR 2012-2013) Pakistan
Dr. Lupituko Luko Mkayula (NR 2012-2013) Tanzania
Prof. Supawan Tantayanon (NR 2012-2013) Thailand
Prof. Vera Ahsen (NR 2012-2013) Turkey
Dr. Gernot Eller (NR 2012-2013) Austria
Dr. Jaroslav Kahovec (NR 2012-2013) Czech Republic

Dr. Gerry P. Moss (*Ex Officio*, as chairman of JCBN) United Kingdom

Appendix B

Suggestion forwarded by Alexander Senning, Professor Emeritus at the Technical University of Denmark *(free translation by Ture Damhus)*

IUPAC could relatively easily, and based on limited funding, become more user-friendly towards clients who need to provide IUPAC names as well as those who need to be able to interpret them. Even though IUPAC, modestly, uses the term 'recommendations', there is a widespread willingness to use IUPAC names if they were easily available.
IUPAC ought to hire professional nomenclaturists, *e.g.* retired CAS employees, who could be paid a basis salary and then per hour of work carried out and who would typically work from at home via the internet.
The large databases using IUPAC nomenclature (*e.g.* NCI, WHO, Wikipedia, Merck Index, medical authorities around the world), could be given bids for revising their entire portfolios of IUPAC names or just new names under preparation or cases where the clients in question are in doubt about how to use particular IUPAC rules.
If one compared with what those database owners spend on maintenance of their information technology systems, the latter would probably dwarf these new nomenclature costs.
The nomenclaturists would at the same time be able to act as an expert panel which could give feedback when there was a conflict between various IUPAC rules, draft new IUPAC rules and check consequences for other rules if a given IUPAC rule was to be changed. They could also investigate beforehand how user-friendly a new rule would be, something which seems to have been traditionally neglected!
Finally, one could have a databank of correct IUPAC names on the IUPAC website to be filled in as new names were generated. In such a database users would perhaps find what they needed before approaching the expert panel.

Appendix C

Boron Hydride Nomenclature Report (M.A.Beckett, April 23, 2012)
[The text here was copied from a PDF file circulated by MB in 2013 and the formatting was partly lost. In particular, reference numbers are not superscript.]

1. Introduction.
This short report summarizes the current position of nomenclature of boron hydride compounds. It briefly reviews the pertinent chapters of the 1990 and 2005 IUPAC publications,[1,2] which in turn draw heavily on the earlier report by Adams.[3] A leading textbook, „Chemistry of the Elements",[4] with an excellent section on boron hydride derivatives also summarizes the salient principles. 'Principles of Chemical Nomenclature, a guide to IUPAC recommendations"[5] was silent on naming of boron hydride derivatives, but the recent 2011 edition[6] contains a chapter in this area. The writing of that chapter has encouraged me to think about (i) possible ambiguities in the current IUPAC systems,[1,2] (ii) the need to update in the light of developments which were noted but not included in these editions, and (iii) advances in the chemistry that have taken place since their publication. My own experience in the area is one of a practising research chemist who worked in the field in the early 1980's. Although my research area has now changed to that of boron oxygen systems, I have maintained an interest in boron hydride derivatives through writing reviews (RSC 'Annual Reports', RSC 'Boron Chalcogen Chemistry') and by attending international conferences featuring boron hydride systems. However, I freely admit to not being an expert in nomenclature, but as a working academic in the area, I can at least alert the committee to possible nomenclature issues. It is more than likely that some, but not all, of these issues might be instantly dismissed by nomenclature experts. I hope this report will raise important questions for further discussion.

2. 'Nomenclature of Inorganic Chemistry, Recommendations 1990'
(1) The report asks for a common development for nomenclature involving boron hydrides with transition-metal carbonyl cluster compounds. I would add Zintl anions to that list as all adopt polyhedral system with related structural descriptors based on electron counting schemes.[7] I am unaware of nomenclature progress in these areas.
(2) The interplay between „stoichiometric" and „structural-descriptor" nomenclature is oversimplified with the result that structural descriptors are undervalued in terms of their potential nomenclature significance. If we take B_5H_9 as an example, it can be named as either pentaborane(9) or *nido*-pentaborane(9). Contrary to the text, the nine H atoms can be inferred from a '*nido*-pentaborane' description,[7] so the *requirement* to state (9) is questionable. However, including H atoms in parenthesis has been conventional practice for many years, and does not detract from the name, and additionally serves the purpose of reinforcing the *nido* structure (as n+4).
(3) The examples cited include the terms *closo, nido, arachno, hypho, klado, conjunto, catena, cyclo* and *commo,* and I assume are all IUPAC accepted. *Endo-* and *exo-* positons are defined to assist in the naming of *nido* and *arachno* systems. Systematic numbering (locants) of deltatahedral clusters are not a problem. The use of μ-*H* is introduced for bridging hydrogen atoms within a name. The hydrogen atom distribution nomenclature system (when used) works for the more open cluster systems *e.g* B_9H_{15} with both bridging and *endo*-terminal H atoms in its *arachno* structure. The footnotes allude to the main problems which need to be addressed which are chiefly related to isomeric species and non-deltahedral cluster geometries *e.g. capped, isocloso, isonido, isoarachno, precloso* and *hypercloso* which have found their way into the chemical literature. *Commo* derivatives and the various modes of cluster fusion need further consideration.[8]
(4) Adduct formation is also a tricky nomenclature problem. The example given, $B_5H_9(PMe_3)_2$, is named as the *quasi*-addition compound: (trimethylphosphine)-*hypho*-pentaborane(9) (2/1). The cluster product is correctly labelled by structure and electron count as *hypho* (more detail on positions of

substitution required). Unfortunately, the choice of this compound does not set a clear example for naming of other adducts. If it were to be named as a true base-acid (2/1) adduct it would need to include the *nido*-term in the acid part of the name, which would be totally misleading. I am of the opinion that the number in parenthesis relates to *actual H atoms present* in the product, but this is not stated explicitly anywhere. Coincidently, there are also 9 H atoms in the *nido*-pentaborane(9) acid, and therefore it is not clear whether the 9 originates from the reactant or product. Adams[3] used actual H atoms present in the acetonitrile adduct of *nido*-decaborane(14), 6,9-$(CH_3CN)_2$-*arachno*-$B_{10}H_{12}$, and named it 6,9-*bis*(acetonitrile)-decaborane(12),[3] but did not use the structural descriptor.
(5) There does not appear to be any issues with nomenclature associated with skeletal substitution (subrogation) and the naming of subrogating atoms or their locations. Again the system for indicating the number of H atoms in parenthesis in the resulting polyhedral species is explicitly defined (although this may add confusion). The decision to include the number of H atoms in parenthesis has a problem with consistency - it essentially treats Group 13 and Group14 hetero systems (e.g carba systems) differently from heteroboranes with heteroatoms from Group 15 or Group 16 which do not have associated H atoms but have *exo* lone pairs.
Group 13 and group 14 derivatives invariably have *exo* H (and sometimes additional *endo* H). Thus the pair of *arachno* compounds 6,9-$C_2B_8H_{14}$ and 6,9-$S_2B_8H_{12}$, are named as dicarba-*arachno*-6,9-decaborane(14) and dithia-*arachno*-6,9-decaborane(12), respectively, even though the cluster frameworks are isostructural and isoelectronic, are both compounds are also related to the bis(acetonitrile) adduct referred to in (4) above.
(6) The section on metallaboranes and metallacarboranes indicates a more detailed approach will appear in a subsequent publication, and a brief footnote relates to hydride ligands which are coordinated to the metal, and how they should be named. I would certainly agree that ambiguities could arise in metallo clusters which contain hydrido ligands on the metal. The example given to illustrate a metalloborane (incidentally chosen as one without a hydride on M) is 6,9-$(Cp^*)_2$-*nido*-6,9-CoB_8H_{12} and is named a dicobalta-*nido*-decaborane(12). I believe, using the method described in the footnote, that the isostructural compounds *nido*-$B_{10}H_{14}$, 6,6,6-(CO)(H)(PPh_3)-6-*nido*-IrB_9H_{13}, and 6,6,6-$(PPh_3)_3$-6-*nido*-OsB_9H_{13} would be named *nido*-decaborane(14), an irida-*nido*-decaborane(14) and an osma-*nido*-decaborane(13). There would appear to be a possible element of double counting of the 6-hydride as and coordinated to the metal centre and as part of the cluster in parenthesis, but interpetation of the footnote is not clear to me. My interpretation is that the three metalladecaboranes cited here all have different H numbers in parenthesis, and yet are all related to the same parent *nido*-decaborane(14). The rule is consistent but the names might be considered misleading without greater detail or structural formula.
(7) The names for polyhedral borate anions and substituted polyhedral borate anions may need a more detailed investigation. Adams has noted that substitution by donor ligands on formally anionic systems can result in neutral (or even cationic) clusters.[3] Should these be named as derived from polyhedral borate clusters? *e.g.* Should the neutral *closo*-1,12-$(Me_2S)_2B_{12}H_{10}$ [derived from *closo*-$[B_{12}H_{12}]^{2-}$ with 2 H^- groups replaced with isoelectronic L groups] be named 1,12-*bis*(dimethylsulfane)-decahydrido-*closo*-dodecaborate(0) or is it a ..dodecaboron?[3] Would a *tris* substituted cationic system be a ...dodecaboron(1+) cation?[3] As a neutral borane derivative perhaps it should be named as such, but the parent borane, formally "$B_{12}H_{14}$", is unknown and I am unsure as to what hydrogen number should be put in parenthesis in such as case. There are also reports of cationic polyhedral clusters e.g. [2,2,3-$(H_2O)(PPh_3)_2$-*closo*-2,1-$PdTeB_{10}H_9(PPh_3)$][BF_4] and the naming of these need further consideration. Again note that this issue is linked to the 'adduct problem' described in (4) again because donor ligands replace *exo* H atoms, to effectively make the LB unit isoelectronic with CH.

2. 'Nomenclature of Inorganic Chemistry, Recommendations 2005'

The recommendations for boron hydride nomenclature for 2005 remain essentially unchanged from those of 1990. The text remains silent on naming of adducts, and non-deltahedral cluster geometries are not commented upon. The 1990 text uses „hydro" for hydrogen atoms, but it now appears „hydrido" is IUPAC preferred.

3. Summary

The systems adopted generally function very well and are robust enough to accommodate most structures. Structural formula of the type 6,6,6-$(PPh_3)_3$-2-Cl-*nido*-6-RuB_9H_{12}, are unambiguous to practising boron hydride chemists. One issue I have found is that many compounds may be correctly named in several different ways by IUPAC methods. The names differ in the level of detail given. Unequivocal names are often very long, and in the interests of brevity are condensed. Ambiguities sometimes unintentionally arise in the condensation process. Full positional substitutional information (including H atoms) might be needed in all cases to achieve unequivocal names. Thus, the longer 2-chloro-6,6,6-tris(triphenylphosphane)-1,3,4,5,7,8,9-heptahydrido-5,6:6,7;8,9:9,10-tetra-μ-*H*-*nido*-6-ruthenadecaboron is a more fuller name for the also correctly named 2-chloro-6,6,6-tris(triphenylphosphane)-*nido*-6-ruthenadecaborane(13). If one names and locates all H atoms, and correctly uses the structural descriptor then the use of the number in parenthesis becomes is redundant. Other important areas which need considering are adducts of neutral boranes and related borane anions, and new structural descriptors.

4. References

1. *Nomenclature of Inorganic Chemistry, Recommendations 1990 (IUPAC Commission on the nomenclature of inorganic compounds*), Chapter I-11, 207-237, Ed. G.J. Leigh, Blackwell Scientific Publications, 1990, Oxford, UK.
2. *Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005*, N.G. Connelly, T. Damhus, R.M. Hartshorn, and A.T. Hutton, Chapter IR-6, 83-110, RSC publishing, 2005, Cambridge, UK.
3. R.M. Adams, *Pure appl. Chem*., **30**, 1972, 683-710.
4.*Chemistry of the Elements*, N.N. Greenwood and A. Earnshaw, Pergamon Press, 1984, 171-177.
5. *Principles of Chemical Nomenclature, a guide to IUPAC recommendations*, G.J. Leigh, H.A. Favre, and W.V. Metanomski (Ed. G.J. Leigh), Blackwell science, 1998, UK.
6. M.A. Beckett, in *Principles of Chemical Nomenclature, a guide to IUPAC recommendations, 2011 Edition*, Ed. G.J. Leigh, Ch.10, 150-157, 2011, RSC, UK.
7. K. Wade, *Adv. Inorg. Chem., Radiochem*., **18**, 1976, 1-66.
8. J.M. Casy, W.J. Evans, and W.H. Powell, *Inorg.Chem*., 1984, **23**, 4132.

Appendix D

Nomenclature Committee of IUBMB (NC-IUBMB) and IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN)

Approved Minutes for the Annual NC-IUBMB and JCBN Nomenclature Meeting

Room 2-33: European Bioinformatics Institute, Hinxton, May 11th 2012

Present: Dietmar Schomburg (DS, Chairman); Richard Cammack (DC, Secretary); Kristian Axelsen (KA); Ron Caspi (RC); Marcus Ennis (ME); Masaaki Kotera (MK); Andrew McDonald (AGM); Gerard Moss (GPM); Ida Schomburg (IS); Keith Tipton (KFT); Hans Vliegenthart (JFGV); Sameer Velankar (SV).

Observers: Ture Damhus (TD, Novozymes A/S and IUPAC Division VIII); Karl-Heinz Hellwich (KHH, IUPAC Division VIII).

Apologies: Athel Cornish-Bowden, Amélia Rauter, Bernardo Herold, Willy Stalmans.

1) The chairman welcomed the participants. He introduced the new members Caspi, I. Schomburg and Axelsen.

2) The agenda was approved.

3) The minutes from the 2011 meeting in Lisbon were accepted, with one correction: the plans for a supplement to the 1996 Carbohydrate Recommendations were introduced by JFGV.

4) There were no matters arising.

5) Reports

   a) Chairman's Report (DS)
   DS introduced the recent activities of the committee, and of the Enzyme Taskforce, most of which are covered in the items below.
   It was agreed that DS' presentation be placed on the internet for future reference.

   DS stressed the importance of maintaining links with IUPAC. The chair of JCBN is ex officio a member of IUPAC Division VIII, Chemical Nomenclature and Structure Representation. A copy of the minutes of the meeting would be sent to the IUPAC Secretariat. (Action: DC)

   b) Treasurer's Report (DC)
   With funding from IUBMB plus support for individual members through IUPAC projects, the committee was within budget in 2011. An additional meeting had been held in November for the Small Molecules Project group.

6) Enzyme Nomenclature and Classification

   a) Report on enzymes classified (DS)

   The enzyme taskforce jointly performs the tasks of assigning new EC-numbers, and updating current entries. Members comprised KFT, GPM, DC, RC, KA, IS and DS. Funding had been obtained for an assistant, Cornelia Munaretto, for two years to work on proposals and draft entries under the guidance of I. Schomburg, but that had now expired. The taskforce had been very active, and 350 new enzymes were entered in the last year, a significant increase from 100-150 per year previously. There were however, up to 3000 potential new enzymes, identified by literature searches, under consideration for classification. Further funding would be needed to maintain the present level of activity of the group.

   b) Issues for classification of particular enzymes (KFT)

      i) KFT noted that there was a need for experts on enzymes acting on nucleic acids, such as those involved in modification of RNA, and also on complex lipids.

ii) Punctuation and capitalization of gene and protein names: there are inconsistencies in biology. According to HUGO (Human Genome Organisation) guidelines, human gene symbols are generally italicised, with all letters in uppercase. Protein designations are the same as the gene symbol, but not italicised. In microbiology the rule is that gene names are in lower-case (although the last letter is often capitalized) italic, while protein names are capitalized. This was not in the remit of JCBN, but it was anticipated that the situation would become more consistent in a few years. Meanwhile, the relevant conventions used in the literature would be applied in the EC list, together with an indication of the species involved if that was not obvious. When referring to an organism, the format "the plant *Ocimum basilicum* (sweet basil)" is to be used.

iii) 'Spontaneous' or 'uncatalysed' reactions

Some enzyme reactions include chemical steps that do not require catalysis by the enzyme. These are currently described as "spontaneous". A postgraduate student had written to point out that, in thermodynamic terms, all reactions occur spontaneously, and that they are better described by 'uncatalysed'. After some discussion it was decided that the present usage did not introduce confusion, and should be retained.

iv) Glossary entries: chemical names used in the Enzyme List are listed in the glossary section of ExplorEnz. Some broad descriptions of substrates were used inconsistently in the "other names", and needed to be combined. For example, the term "fatty aldehyde" may be given as a synonym of "long chain aldehyde". Moreover, some substrates used in assays of enzymes of broad specificity such as "versatile peroxidase", do not occur naturally. These need clarification, with links where appropriate to KEGG and ChEBI. Action: ALL

v) Enzymes in "Limbo": These are enzymes for which there is, as yet, insufficient information for listing. McDonald was keeping a list in DraftEnz, pending further information becoming available. They can be accessed by reviewing the "dormant" entries.

vi) Dirigent proteins are proteins without catalytic function, but which guide the configuration of the products of enzyme-mediated reactions. They were not classified as enzymes, but at some stage it would be necessary to decide how they should be referred to in enzyme descriptions. No action at present.

vii) Enzyme.me.uk is a database, originating from Russia but hosted in Germany, that contains unacknowledged use of the EC list. Further, it claimed copyright on the material. Since the EC list is copyright IUBMB, DS would write to Willy Stalmans, the Chairman of the IUBMB Committee for Publications, to inform him of the situation and ask him to take action.

7) IUPAC project reports

a) Nomenclature of Flavonoids

Hellwich summarized recent progress. Meetings had been held in 2011, in Lisbon and San Juan and in 2012 in Hinxton. The minutes of the recent meeting, prepared by IS, were tabled. Recommended names were being created for the major classes. These were based on parent compounds; some preferred trivial names were included but they were not designated as preferred. Herold had written a "Newcomers' Guide" for name construction. Another meeting of the Group was planned to be held in September in Lisbon.

b) Glossary of Small Molecules of Biological interest

DC described progress with the list of compounds, selected for being important biologically, and which presented issues of nomenclature. The final document would comprise about 300 diverse compounds, representative of groups that are frequently cited in the literature. The glossary would explain their biological interest and provide links to existing IUPAC documents. An internal database had been constructed by McDonald, which could display molecular details and structure, and biological importance. Entries would be described consistently, using a controlled vocabulary.

c) Revision of carbohydrate nomenclature

JFGV anticipated that a draft project proposal would be produced by the end of the summer. This would include glycosides, but not flavonoids. It would not be possible to generate a short document.

d) TD described recent developments in IUPAC Division VIII.

TD also explained that Division VIII was not happy with the uncontrolled vocabulary seen in IUPAC nomenclature recommendations, where numerous terms such as 'common', 'accepted', 'trivial', 'discouraged', 'not encouraged', 'not included in these recommendations', 'deprecated' and so forth are being used without a clear definition. This had led to a suggestion in Division VIII to work at establishing a document on 'Nomenclature Terminology'.

8) Codified chemical terminology

A group in Denmark, including school teachers, had found that the present entries in the Gold Book were somewhat inconsistent in a number of important cases. This had fostered, to begin with, the pilot project on ontologies that was reported to JCBN at the meeting in Copenhagen in 2008 and also in the article in *Chemistry International* Vol. 31, No. 5, pp. 6-11, September-October 2009. Currently, the group was working on systematisation of the terminology already published in a Danish handbook of chemical terms for students. The contents of the book had been entered into a professional terminology program designed for working with ontologies.

9) Update on Action Items from the Minutes of the 2011 Meeting

a) Commemorative article for the 50th anniversary of the Enzyme List.

Because of pressure of other work, there had been no further developments.

b) Vectorial enzymes: use of “side 1” and “side 2”

This proposal was being implemented in the Enzyme List by AM.

c) EC classifications for artificial mutant (engineered) enzymes with novel activities

This was discussed in the meeting of the EC Taskforce. There was concern that it might generate a large number of EC numbers, which would require much time and effort and also would hinder the use of the Enzyme List for tracing physiological pathways. It was suggested to make a new parallel list for such enzymes (or “chemzymes”) as well as ribozymes and other non protein-catalysed reactions. However, it was pointed out that currently the required resources for such a parallel list are not available. A comment was made by DC that if companies want EC numbers for engineered enzymes, for patent reasons, they should pay for them. However TD stated that companies might well not want EC numbers for engineered enzymes, in particular for regulatory reasons.

d) Version number for the EC list. This functionality is provided by a log of all changes in DraftEnz and ExplorEnz.

10) Membership of the committee

At the 2011 meeting DS had announced his intention to resign as Chair of the committee, but continue as a member. This was agreed. GPM was elected unanimously as his successor, and took over the rest of the meeting.

GPM thanked DS for his leadership for the past five years and work as Chairman. This was endorsed by the whole committee.

KHH and TD were elected Associate Members, which would strengthen the connection between IUPAC Division VIII and JCBN.

DC was to stand down as Secretary. He agreed to stay in post for one year to assist his successor, who was to be decided by DS and GPM after further discussions. Later, RC agreed to be nominated.

KFT would continue as Joint NC-IUBMB and JCBN member

JFGV would transfer from Titular member to Associate member of NC-IUBMB and JCBN; to be supported by the prospective IUPAC project on Carbohydrates.

Associate members:

Database representatives: SV stated that Helen Berman had asked to continue as principal representative of the Protein Databank.
MK was to be database representative for KEGG, along with Minoru Kanehisa.

AM, who is currently an associate member, is to become a titular member of NC-IUBMB.

Donald Nicholson† and Minoru Kanehisa were nominated as Emeritus members.

GPM requested updates for the committee mailing circulation list. (Action: All).

11) Any Other Business

TD mentioned the recent publication of the second edition of "Principles of Chemical Nomenclature". The biochemical section had been written by GPM, featuring new sections on nucleic acids and vitamins. KHH offered to send an information leaflet on this book as PDF file.

IUPAC was also creating short (2-4 page) documents on "Essentials" of different areas of Nomenclature. Documents being worked at cover polymers, organic and inorganic nomenclature. The committee was asked to consider a possible Essentials document introducing biochemical nomenclature (Action: All).

GPM drew attention to the list of IUPAC Bibliographic Sources at
http://www.chem.qmul.ac.uk/iupac/bibliog/

12) Date and Place of Meeting in 2013

KFT invited the committee to meet in Dublin.
Possible dates May 13 – 15 or May 27 – 29, depending on availability.

13) Open Forum Presentations

Syed Asad Rahman (European Bioinformatics Institute) made a presentation on EC-Blast, a program to map and compare chemical reactions. It could deal with all classes of enzyme reactions, including lyases.

†Immediately after the meeting, the committee was informed that Dr Nicholson had died on May 12.