

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

Minutes, meeting of Division Committee
Glasgow, UK, 31 July–1 August 2009

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

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

Titular members

Jonathan Brecher (USA) **JB**
Kirill Degtyarenko (UK) **KD**
Stephen R. Heller (USA) **SRH** (only part-time)
Karl-Heinz Hellwich (Germany) **KHH**
Philip Hodge (UK) **PH**
Alan T. Hutton (South Africa) **ATH**
G. Jeffery Leigh (UK) **GJL**
Jeffrey Wilson (USA) **JW**

Associate members

Jaroslav Kahovec (Czech Republic) **JK**
Alexander Lawson (Germany) **SL**
Ebbe Nordlander (Sweden) **EN**

József Nyitrai (Hungary) **JN**
Warren H. Powell (USA) **WHP**
Andrey Yerin (Russia) **AY**

National representative

Jan Reedijk (Netherlands) **JR**

Observers and guests

David StC Black
(Australia, IUPAC secretary general; in part) **DStC**
Michael J Scott (USA) **MJS**
Arthur Maximenko (Belarus) **AM**
Michelle Rogers (USA; young observer; in part)
Dmitrii Perepichka (Canada; young observer; in part)
Amélia P. Rauter (Portugal; in part) **APR**
Bryan Pearson (USA; IUPAC secretariat; in part, see item 11) **BP**
CCE: Eva Åkesson (Sweden), Peter Mahaffy (Canada) (see item 14.1)
COCI: Mark C. Cesa (USA), Michael D. Booth (South Africa) (see item 14.2)

The complete Division VIII Committee membership as of July 2009 is given in Appendix A.

1. Introductory remarks and housekeeping announcements.

In addition to practical information on internet access, registration and times for lunch breaks, *etc.*, it was announced that secretary general David StC. Black was planning to visit the Division during the day.

2. Received apologies for absence.

Hervé Schepers and Md. Abul Hashem were not able to attend.

3. Introduction of attendees.

SL announced that he now works for Elsevier Properties, a Reed Elsevier company, and not directly part of Elsevier. His new E-mail address is alexander.lawson@reedelsevier.ch.

Arthur Maximenko is a colleague of Jonathan Brecher in CambridgeSoft.

In addition to the division members in attendance, Prof. David StC. Black participated in large parts of the meeting. Young observers Michelle Rogers and Dmitrii Perepichka participated part-time.

4. Approval of agenda. A few more new projects were added to the list under item 8.9.

5. Minutes of meeting in Büdingen, Germany, 31 July–1 August 2008.

The draft of March 15, 2009, was approved with a few minor corrections. (The minutes have since been made available on the IUPAC website.)

6. Matters arising. ATH mentioned that the Hungarian translation of the 2005 *Red Book* (Büdingen minutes 2008, item 13.1) carries no reference to the authors of the original publication. JN to bring this up in ICTNS.

GPM mentioned that the wolfram/tungsten issue would be brought up during the Committee meeting (see item 15.2). Also, the naming of Uub was to be discussed (again, see item 15.2).

7. Recommendations, translations and related publications since 2008 Division Committee meeting.

7.1 Nomenclature for rotaxanes and pseudorotaxanes (IUPAC Recommendations 2008), A. Yerin, E.S. Wilks, G.P. Moss, A. Harada, *Pure Appl. Chem.* **80**(9) 2041-2068 (2008). A German translation has appeared: Nomenklatur der Rotaxane und Pseudorotaxane (translated by I. Schomburg), *Angew. Chem.* **121**, 4719-4738 (2009).

7.2 *Compendium of Polymer Terminology and Nomenclature* (IUPAC Recommendations 2008) "*Purple Book II*" (Eds. R.G. Jones, J. Kahovec, R. Stepto, E.S. Wilks, M. Hess, T. Kitayama, W.V. Metanomski; RSC Publishing 2009)

7.3 G.J. Leigh: Periodic Tables and IUPAC, *Chem. Int.* **31** (1) 4-6 (2009).

7.4 K.-H. Hellwich: *Chemische Nomenklatur – Die systematische Benennung organisch-chemischer Verbindungen* [Chemical nomenclature – the systematic naming of organic-chemical compounds] (3rd Ed., Govi-Verlag 2008).

7.5 *Kemisk Ordbog* [Chemical Dictionary] (3rd Ed., Eds. T. Damhus, S. Møller, A. Senning; Nyt Teknisk Forlag, 2008). A guide to the Danish adaption of IUPAC nomenclature recommended by the Danish Chemical Society.

7.6 Glossary of class names of polymers based on chemical structure and molecular architecture (IUPAC Recommendations 2009), M. Barón, K.-H. Hellwich, M. Hess, K. Horie, A.D. Jenkins, R.G. Jones, J. Kahovec, P. Kratochvíl, W.V. Metanomski, W. Mormann, R.F.T. Stepto, J. Vohlídal and E.S. Wilks, *Pure Appl. Chem.*, **81**(6), 1131-1186 (2009).

7.7 S.R. Heller, A.D. McNaught: The IUPAC International Chemical Identifier (InChI), *Chem. Int.* **31** (1) 7-9 (2009).

The secretary had noted that publications 7.1 and 7.6 were *not* mentioned under *Recommendations* and publication 7.2 was *not* mentioned under *Publications* on the IUPAC web site.

KHH mentioned that publication 7.6 will be translated in part into German and published in *Angew. Chem.*

8. Division VIII projects [note: project numbers do not always correlate with numbers given on the IUPAC website].

8.1 IUPAC International Chemical Identifier (InChI) – report from the InChI subcommittee (2007-052-1-800).

SRH reported on the status of the InChI project, in particular the establishment of the InChI trust. Formally, the InChI Trust was incorporated in the UK as a private company with the company number 6906661 on May 15, 2009.

The InChI subcommittee had had a meeting just the day before the division meeting. Later, the minutes from that subcommittee meeting have become available on the division webboard. They are included here as Appendix B.

Other sources of information on the InChI project are the 21 July 2009 press release on the IUPAC homepage, and the article in *Chemistry International* **31** # 5 (2009) 16.

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

Chapters 1, 2, 3, 7, 8 and 10 had been available for review on the webboard for a while. WHP reported that there were still a few issues being worked in sections P-44 (seniority of parents) and P-45 (selection of PINs). A few other issues remaining in chapters 5, 6 and 9 were mentioned. A discussion of the use of locants followed (when can locants be left out, the use of 'per', locants vs. parentheses, etc.). CAS more or less always uses locants. Several attendees were in favor of reducing locant usage when possible. Section P-14.3.4 will discuss omission of locants. The name 2-chloroethan-1-ol will for sure be a P-name.

The review process will continue as the remaining parts are posted on the webboard. Small corrections should be sent to WHP directly, whereas matters of principle can be brought up on the webboard.

TD pointed out that the Appendix dealing with substituent groups is very important and should be made available as soon as possible. WHP said the Appendix was currently with Henri Favre.

The review process was foreseen to run through 2010, with the advisory subcommittee being eventually involved and then ICTNS. Publication should be a reality in 2011.

8.3 Rotaxanes (Project 2002-007-1-800).

Published, see 7.1. Reprints were available at the meeting.

8.4 Cyclic peptides (2004-024-1-800). GPM had no progress to report.

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

GPM had no progress to report.

8.6 Comparison of procedures for naming hydro derivatives of fused ring systems.

WHP had no progress to report.

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

GJL reported about the meetings held since last, in Cambridge in April 2009 and in Glasgow just before the Division Committee meeting. All chapters of the book had been drafted by now, and the plan was now to have all chapters finished by the end of 2009 for review by anybody interested. Regarding publication, GJL was happy to approach RSC first. The color of the book was an unresolved question. The book will go via ICTNS, but GJL stressed that there will be no new nomenclature in it. The IUPAC secretariat is still getting inquiries for the first edition of the book.

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

RMH reported from the project group meeting held in Glasgow the day before the Division Committee meeting.

WHP had been present, which had enabled some useful discussions.

There had been discussion of the timescale for the project (scheduled to finish end 2010) and the milestones included in the project proposal – which had proven not to be practical as the issues identified for publication of recommendations had proven to be inextricably intertwined. The timescale means that there is some pressure to make decisions on the PINs procedure. However, even deciding on *the kind* of PINs for compounds based on elements from various groups had proven problematic, and the decision made at the Buedingen meeting of the Division Committee was revisited. There were ongoing issues with compounds of Ge, Sn, Pb, Sb, and Bi in relation to our perceptions of the kinds of name that the communities at large might prefer.

Significant advances were made in discussion with WHP in relation to the need to use additive nomenclature for systems where charge is delocalised, where neutral non-substitutable groups are bound to another atom, and where bonds are delocalised (other than for delocalised parents). There are still some issues to be resolved around oxoacid-based names vs. substitutive names based on parent hydride 'ane' names; and regarding choice of central atoms in ring and chain structures that contain only main group elements. A document clarifying kappa and eta grammar will also be prepared. Clusters loom ahead as a complex and basically untouched subject. Adducts and solvates need to be coordinated with the Blue Book section on similar compounds.

8.9 Macromolecular projects (with Division IV).

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

PH reported. The task group leader is Prof. T. Kitayama. Whilst some progress had been made since last year, the project was still only nearly complete.

8.9.2 Nomenclature for Chemically Modified Polymer Molecules (1999-051-1-800).

PH reported. Task group leader is also here T. Kitayama. This was approved as an interdivisional project. It is mainly 'nomenclature', although some parts have a 'terminology' aspect. The project had not been discussed in

detail for about 2 years. The subcommittee for polymer terminology (of which T. Kitayama is the secretary) was only to meet two days later.

8.9.3 Nomenclature for Polymer Rotaxanes [website says 'Rotaxane Polymers'] (2007-009-1-800).

AY pointed out that the chair is J. Vohlidal. The project had been waiting for 8.3 to be finalized and there was no progress to report.

8.9.4 Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers (2001-081-1-800) [two documents]. JK was critical of the decision to produce two papers. JK will send a corrected version of the manuscript to GPM; then it will be posted on the webboard. [Secretary's remark: the information on the webboard is not updated. The chair is still listed as the late V. Metanomski.]

8.9.5 Preferred Names for Polymers – List of preferred, acceptable (other IUPAC-approved) and not acceptable (ambiguous, wrong or outdated) names for polymers (2008-015-1-400) [project number was missing in the agenda].

The purpose is to prepare a list of all names of polymers and constitutional units published in IUPAC documents and to classify the names in this list as preferred, acceptable and not acceptable (outdated/obsolete, ambiguous or wrong). Outcome should be a publication in PAC which clarifies which of the - in some cases many - different names are still recommended.

After approval of the project in early summer 2008, the task group chairman, Prof. Werner Mormann, and KHH had developed a concept for a relational database which was intended to help in the systematic extraction of all names for polymers and constitutional units of macromolecules ever published in IUPAC documents. This concept was given to a programmer who provided a beta version of the database program only a few days before the Glasgow meeting

GMP asked about source-based names for copolymers, but KHH told that the project is primarily about structure-based names. Thus only constitutional repeating units need to be given preferred names. KHH pointed out that existing rules only give a clear instruction on how to determine the constitutional units as the basis for naming. The result is a unique structure (sequence of constitutional units) to be named. But for many constitutional units there is more than one possibility for naming them, and these different possibilities have been favoured differently at different times.

It was suggested that for structure-based names, the group names recommended in organic nomenclature must be used. KHH replied that polymer nomenclature has specific requirements which in several cases will lead to another name for a group. For example, the general rule in structure-based nomenclature is to name groups not part of the backbone always as substituents. This results in the name 1-methylethylene rather than propane-1,2-diyl when this group is a repeating unit.

KHH and GPM stated that as nomenclature project it should be published as Division VIII with Division IV rather than the other way round. (But the project number is actually Division IV.)

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)

PH is the task group leader. The project has been running for 1 year now and has another year to go. Progress had been modest until now, but the day before the Division VIII meeting, the group had had an excellent meeting. (This was to be followed by another meeting after the Division VIII Meeting). The project is likely to be completed on time.

8.9.7 Basic guidelines to polymer nomenclature (2008-032-1-400). KHH reported. The project group was to meet later in Glasgow. The chairman is Dr. Roger C. Hiorns.

8.10 Other interdivisional projects.

8.10.1 Classification, terminology and nomenclature of borophosphates (2003-034-1-200) [with Division II]. No news to report.

8.10.2 Recommendations for nomenclature and databases for biochemical thermodynamics (2006-023-3-100). The document was currently under discussion between JCBN and ICTNS. There are differences of view between physical chemists and biochemists within this subject. It is hoped that the issue may be resolved through collaboration between Division I and JCBN in 2010.

9. Future projects/activities.

9.1 Graphical representation of reactions. No news was reported. Bill Town was not present.

9.2 Stereochemical notation in polymers. KHH just a few days earlier had drafted the project proposal which was now being looked at in the prospective project group. The project involves updating the *Pure Appl. Chem.* **53** (1981) 733-752 document on stereochemical terminology.

9.3 Graphical representation of polymers. KHH reported. There had not been anyone volunteering to work at this until now. The subject was excluded from the now completed project on graphical representation standards, and perhaps there was a bit of funding left from that project. The 1994 document is not in accord with the new graphical representation document.

9.4 Metallacycles. No progress to report, but it was anticipated that once the inorganic PINs project has advanced a bit further it will be natural to start work on the clusters, a subject related to metallacycles. MJS pointed out that clusters are a very complex subject. It was noted that Chemical Abstracts define clusters to be assemblies of metal atoms with 13 or more metal atoms linked by direct metal-to-metal linkages. GJL stressed the need of having an ongoing activity in the area. TD recalled the interest in clusters from former member of the Commission on Nomenclature of Inorganic Chemistry, Prof. Andreas Dress (a mathematician), and TD agreed to check the network to see if any younger colleagues of Dress would be available now and interested in working on clusters.

9.5 Boron nomenclature. It was pointed out that there might be synergism between the project on clusters and the subject of boron hydrides. Mike Beckett should be approached regarding boron nomenclature.

9.6 Proposal by L. Öhrström (2009-012-1, Coordination polymers and metal organic frameworks: nomenclature guidelines).

There was some discussion of the review process in general and the need to clarify roles with the secretariat.

9.7 Proposal by APR (2009-018-1, Recommendations on Nomenclature of Flavonoids). APR was present during the discussion of this item. KHH underlined the need for a specific document for the flavonoid community.

Nomenclature needs attention, *e.g.* when it comes to complicated branched flavonoids.

9.8 Division VIII activities in the International Year of Chemistry (2011). The committee brainstormed about this and reported the ideas generated under item 14.1. Keywords for these ideas are listed in Appendix C. Everybody was urged to sign up on the 2011 homepage (<http://www.chemistry2011.org>).

9.9 Other possible projects. Keywords:

- delocalized charges; KHH will circulate 1981 draft document by D. Hellwinkel [now available from the secretary as well]
- stereonomenclature of rotaxanes/catenanes; AY will make proposal; stereochemical terminology must be reviewed/revised
- small molecules of key importance in biochemistry (examples could be ATP and coenzyme A); Richard Cammack will be involved
- metal clusters scoping exercise by MJS and RMH; MJS will try to contact metal cluster chemists at ACS conference.

10. Membership.

10.1 Status of committee membership (membership at time of meeting, see Appendix A).

The Committee started by noting with sadness the decease in December 2008 of Val Metanomski [cf. *Chem. Int.* **31** (2) (2009) 17-18 + 19] and the recent passing of Alan Sargeson [cf. *Chem. Int.* **31** (2) 19 (2009)], former chairman of the Commission on Nomenclature of Inorganic Chemistry.

SL ends his term as associate member, SRH ends as titular member.

AY becomes titular member.

Elected for associate membership 2010-2011: JK, KHH, EN, JN, WHP, JR.

APR (Portugal) will be a new national representative. There was some confusion about certain of the other elections of national representatives, but they do seem to be correctly listed now (February 2010) on the IUPAC webpage.

It was noted that national representatives have not been very active in the past. DStC suggested Division VIII should be more proactive in relation to the national representatives. RMH had some ideas for perhaps interacting with delegates at Council meetings.

GJL will represent Division VIII in ICTNS.

10.2 Advisory subcommittee.

The membership needs to be updated. Ted Godly was mentioned as a possible member, as was Jörg Pabel from the University of Munich (suggested by KHH).

11. Webboard(s).

DStC introduced BP, the most recently employed member of the IUPAC secretariat staff. BP gave a presentation on how to work with the Division VIII discussion board, one of a number of member forums created for the various IUPAC division and standing committees and working groups and available via the IUPAC website.

One important thing to note is that one may customize the display mode.

BP can erect new fora for working groups, *e.g.* for the Division VIII Advisory Subcommittee, and is very willing to do so. It was mentioned that some problems encountered by members trying to navigate in the forum might be browser-dependent. There have also been invalid E-mail addresses in the system so that members have failed to receive alert messages when items were posted in the forum.

Inquiries regarding access to the forum and problems encountered may be sent to iupachelp@iupac.org.

12. Publicity

12.1 IUPAC and IUBMB nomenclature web site. GPM handed out a sheet showing the statistics of usage as of July 2009, but it was stressed that there are significant seasonal variations (depending on *e.g.* the onset of the academic year), so that a comparison between the 2008 and 2009 data would not be fair at this time.

12.2 IUPAC website.

There are still items that are only on the old website. FIZ-Chemie has been very collaborative, but there is nobody overseeing the work carried out by the Prague group. SRH said the problem of the unsatisfactory function of the website must be solved at high level in IUPAC.

12.3 Other publicity issues. Regarding journals, GPM said that editors do not want papers to be delayed because of nomenclature matters. The RSC and other editorial offices do not have staff who can correct nomenclature.

13. Reports from other bodies.

13.1 Committee on Chemistry Education (CCE). RMH reported. CCE is involved in the management committee for the International Year of Chemistry 2011. In 2008, there was a conference on chemical education with the theme 'Chemistry in the IT age', whereas the next conference was to have a theme about chemistry's role in the global sustainability age. RMH said CCE was very willing to review the *Principles* text (*cf.* item 8.7).

13.2 Committee on Printed and Electronic Publications (CPEP). The meeting had not yet been held. SRH pointed out that with his exiting the Division Committee, a new liaison to CPEP would have to be found.

13.3 Committee on Chemistry and Industry (COCI). The Committee had not yet met (but see item 14.2).

13.4 PAC Editorial Board. The board had not yet met at the time of the Division VIII meeting. Later, GPM submitted the following: The main item discussed which will affect Division VIII is the style of publication of technical reports and recommendations. In future these will be published in the same style as a research paper or review. This is with the title, authors and affiliation followed by the text. The long lists of working parties, Division membership, *etc.* will be published as footnotes at the end.

13.5 Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS). Nothing particular to minute.

13.6 Report of JCBN meeting in Braunschweig (GPM/KHH). The funding for Sinéad Boyce ran out in January 2009, and Richard Cammack is new secretary for JCBN for 1 year. Cammack is also lead person in the small molecules project. The meeting had dealt with matters of enzyme nomenclature/problems with the enzyme list, and update of the carbohydrate document (one or two documents?). The Braunschweig minutes are included as Appendix D.

14. Visits from other committees.

14.1 Visit from CCE (Committee on Chemical Education). E. Åkesson and P. Mahaffy from CCE gave a presentation of current activities in CCE.

RMH, the Division VIII representative in CCE, was commended for his work as an associate member in CCE.

CCE priorities include curriculum considerations, in particular learner-centered education; public understanding and appreciation of chemistry with a focus on ICY2011; the connection between chemistry and sustainability; chemistry and ethics. There is a biannual conference on Chemical Education in which CCE is heavily involved.

CCE is very global in its membership, and it was stressed that IUPAC must ensure global participation in IYC2011. A number of countries had sponsored the initial IYC2011 resolution, but it is important to get the remaining countries involved.

A discussion of the ideas generated by CCE and the ones mentioned above under item 9.8 followed.

In connection with TV shows it was mentioned that Adam Hart Davis in the UK has chemical background. H. Kroto is establishing an archive. One could make a collection of the "100 most important chemical papers". Stress understanding of the different perspectives of the macroscopic and the microscopic world. With respect to nomenclature one could have a look at chemical names in newspapers, on labels found in the supermarket *etc.*

14.2 Visit from COCI (Committee on Chemistry and Industry). M. Cesa presented COCI's terms of reference and highlights of current activities. These include the IUPAC-UNESCO-UNIDO safety training program, public appreciation of chemistry, managing the IUPAC Company Associates and preparing for the 2012 International Conference on Chemicals Management. Cesa also mentioned the Strategic Approach to International Chemicals Management (SAICM).

15. Any other business.

15.1 Proposal by P.G. Nelson regarding the periodic table (posted on Division VIII webboard May 26, 2009). GJL was of the opinion that IUPAC should stick to what we have (*i.e.*, the 18 groups periodic table) – it is generally accepted. In any case, it was generally acknowledged that: IUPAC cannot control periodic tables around the world; IUPAC is not entitled to 'give permission' to do this or that; and IUPAC will not endorse particular proposals. GJL to reply to P.G. Nelson.

15.2 Other.

- JR reported from Division II. Regarding element 112, it was clear that there were arguments against the atomic symbol Cp, and this was to be communicated to the discoverers. As for the wolfram-tungsten discussion, the case was now closed. Details can be found in JR's report inserted here as Appendix E.

- GJL brought up the issue of ensuring continuity in IUPAC work dealing with the color books. This entailed a lively discussion. RMH said we should perhaps adopt a strategic view of all the color books. ATH suggested it could be a standing item on the Division's agenda. KD asked whether one could make the color books into 'living documents'. GPM said it might be an idea to have a newsletter.

Comments from the community could be accumulated by the secretary or another officer.

There ought to be a repository for final versions of manuscripts in Division VIII.

We must make sure the Blue Book is preserved once it is published.

Discussion of moderator/review processes.

DStC was not sure about the economy in all these suggestions, but said we need 'apprentices' for each area of nomenclature to ensure the continuity. RMH suggested that apprentices be designated for each of the Color Books and that the president handle any questions regarding the future of the Color Books together with the apprentices. MJS was designated apprentice for the Red Book; JB for the Blue Book and graphical representations; and KHH preliminarily for the Purple Book.

- KHH took up the question of how to deal with names that are still around in certain IUPAC publications but are not in accord with current recommendations for systematic names (examples could be 'phosphonium' and 'ethanolamine'). One place where it is important to be able to classify such names in a clear and consistent way is in *Principles* (cf. item 8.7).

TD reminded about the decision to only use three adjectives for names: *acceptable*, *not acceptable* and *preferred*, eliminating the earlier multitude of not very helpful descriptions such as 'deprecated', 'not encouraged', 'not included in these recommendations', *etc.* This usage was adopted in the paper on graphical representation standards and according to TD, the Red Book authors had at least tried to use it, if not with complete success.

It was agreed that TD try to rephrase the Blue Book introduction so as to encompass this thinking and place the resulting draft on the Division webboard.

The name 'graphene', already very established in the public, was mentioned by PH.

As a final practical remark, TD asked that correspondents strive to give their E-mail messages informative subject titles. Typically replies to messages carry the original message's title, and long series of E-mails eventually accumulate in one's folders that deal with anything else than what is in the subject line, making searches rather difficult. [TD remark: the secretary has a folder of almost 3000 E-mail messages dealing with Division VIII and general IUPAC matters.]

16. Date and time of next meeting.

EN had volunteered to arrange the meeting to take place in Lund, Sweden. The dates 14-15 August were mentioned as probable dates. It was mentioned that a Saturday/Sunday or Sunday/Monday meeting was preferable.

17. Adjourned.

Appendix A

Division VIII Committee, membership as of July 18, 2009 (as listed on the IUPAC website)

Gerard P. Moss (United Kingdom)

President

Richard M. Hartshorn (New Zealand)

Vice President

Ture Damhus (Denmark)

Secretary

Titular Members

Jonathan Brecher (United States)

Kirill Degtyarenko (United Kingdom)

Stephen R. Heller (United States)

Karl-Heinz Hellwich (Germany)

Philip Hodge (United Kingdom)

Alan T. Hutton (South Africa)

G. Jeffery Leigh (United Kingdom)

Jeffrey Wilson (United States)

Associate Members

Jaroslav Kahovec (Czech Republic)

Alexander Lawson (Germany)

Ebbe Nordlander (Sweden)

József Nyitrai (Hungary)

Warren H. Powell (United States)

Andrey Yerin (Russia)

National Representatives

Farzana Latif Ansari (Pakistan)

Youngkyu Do (Korea)

Ivan L. Dukov (Bulgaria)

Md. Abul Hashem (Bangladesh)

Lauri H.J. Lajunen (Finland)

Hiroshi Ogino (Japan)

Jan Reedijk (Netherlands)

Ex Officio

Dietmar Schomburg (Germany)

Joint Commission on Biochemical Nomenclature

Appendix B

IUPAC Division (VIII) of Chemical Nomenclature and Structure Representation International Chemical Identifier (InChI) Subcommittee

Minutes of the meeting on 30th July 2009 at the Crowne Plaza Hotel, Glasgow, UK

Present: *Subcommittee members:*

Steve Heller (Chairman)
Evan Bolton (US National Center for Biotechnology Information)
Sandy Lawson (Elsevier, Frankfurt)
Alan McNaught (Secretary; InChI project coordinator, Cambridge, UK)
Igor Pletnev (ex-officio developer) (Moscow State University)
Tony Williams (ChemSpider)
Andrey Yerin (Advanced Chemistry Development, Moscow)

Observers:

John Barnard (Digital Chemistry Ltd)
David Black (IUPAC Secretary General)
Colin Bulpitt (Taylor & Francis)
Kirill Degtyarenko (IUPAC Division VIII)
René Deplanque (FIZ-Chemie, Berlin)
Richard Kidd (Royal Society of Chemistry)
Rachel Kirton (Taylor & Francis)
Dave Martinsen (American Chemical Society)
Tim Miller (Thomson Reuters)
Hinnerk Rey (Elsevier, Frankfurt)
Ulrich Roessler (FIZ-Chemie, Berlin)
Dick Wife (SORD B.V)

Apologies:

Subcommittee members:

Colin Batchelor (Royal Society of Chemistry)
Marc Nicklaus (US National Cancer Institute)
Steve Stein (NIST)
Chris Steinbeck (European Bioinformatics Institute)
Keith Taylor (Symyx Technologies, CA)
Dmitrii Tchekhovskoi (ex-officio developer) (NIST)
Graeme Whitley (Wiley, New York)
Jason Wilde (Nature, London)

1.0 Minutes of the previous meeting

The minutes of the meeting in Salt Lake City on March 23rd 2008 were approved without comment.

2.0 InChI Trust status

Copies of the current Business Plan and the InChI Trust logo were circulated.

2.1 Background and current position

Steve Heller gave a brief overview of the status of the InChI project. The initial collaboration between IUPAC and NIST had had been remarkably successful; however NIST had taken the development of the Identifier to the point at which its needs were largely satisfied, and did not wish to provide resources for further development. There had been a need to find other sources of funding, for maintenance and for continuation of the project to deal with areas of chemistry not currently covered. Also it was apparent that the community of InChI users and potential users wished to see InChI maintenance and development placed on a firm business basis as a stable operation; it had become clear that this would be difficult to achieve under the auspices of IUPAC alone. The InChI Trust had been set up to address these concerns. Authority for the InChI standard would continue to be provided by IUPAC through the Division VIII InChI Subcommittee, and the Trust would be responsible for implementation of community requirements as approved by the Subcommittee.

Chemistry publishers in the UK (Nature and the Royal Society of Chemistry) had been the first to offer funding support for the Trust. RSC had provided administrative facilities to enable the Trust to be incorporated in the UK, and an application had been made for charitable status. Offices and computer facilities for the Trust had been provided free of charge by FIZ-Chemie Berlin Other organisations (Taylor & Francis, Symyx Technologies, OpenEye) had subsequently joined the Trust, and very recently final agreement to participate had been received from Thomson Reuters and Elsevier. Steve Heller would continue his publicity and awareness-raising activities in order to attract additional membership. It was intended to continue the development of InChI under the auspices of the Trust as a IUPAC-approved open-source algorithm, to be made freely available to the community for use as they see fit.

The Business Plan contained budget estimates for a five-year period; it was expected that the need for continuing development would decline after a few years and that funding requirements would eventually reduce to maintenance level. It was intended that all work would be carried out under contract: there would be no employees. Steve Heller would act as part-time Director, Igor Pletnev would continue as developer, and other developers would be added as required. It would be particularly important to spread knowledge of the InChI algorithm amongst several people, to ensure stability and continuity. It was noted that the logo currently displayed in the Business Plan was not that finally approved by the Trust Board.

Requirements for development would be established by the IUPAC InChI Subcommittee, working through appropriate subgroups; at present there were groups on requirements for organometallic structures, InChI/InChIKey resolver protocol, business rules for structure input control, and the use of InChI in description of chemical reactions.

The first meeting of the InChI Trust Board would take place on September 11th in Cambridge UK, and invitations to attend would be issued soon.

Steve Heller tabled his InChI report to IUPAC Division VIII for inspection.

2.2 Relationship with the American Chemical Society

Steve Heller had made contact with ACS on several occasions in connection with InChI, most recently in March of this year, and had recently received a message from Publications Division in response to the press release announcing launch of the InChI Trust. Dave Martinsen outlined some of the concerns expressed:

2.2.1 *Continuing role of IUPAC as standards body*

There was some doubt as to whether the continuing role of IUPAC as standards-setting body for InChI was assured. For example, diagrammatic representations of relationships between various bodies could be taken to imply that IUPAC was being side-lined. Steve Heller emphasised the crucial role of the Division VIII

InChI Subcommittee in this connection. All developments would need the approval of this body for incorporation in the InChI standard. It was therefore of prime importance for IUPAC to continue funding the Subcommittee at an appropriate level. Alan McNaught pointed out that the standard would lose all credibility if not authorised by IUPAC. It was agreed that the Business Plan and future documents on InChI development should give more emphasis to IUPAC's role.

2.2.2 *IUPAC participation in the InChI Trust*

It appeared that IUPAC was not at present participating directly in the Trust. Dr McNaught thought that an invitation for IUPAC to join as funding participant had been sent to IUPAC, but it appeared that this was not so; an invitation would be issued for consideration by the IUPAC Executive in October. Furthermore ACS considered that IUPAC should have an official role on the InChI Trust Board regardless of any paid-up Trust membership; this idea was supported and would be recommended to the Board meeting on September 11th. It was noted that the Trust's Articles of Incorporation were drawn quite widely, as is normal for such documents, but the primary objective was clearly specified as development and maintenance of the InChI standard.

David Black emphasised that IUPAC was delighted that the Trust had been established, though it would have been preferable for the set-up to have been carried out in a more independent way, through the IUPAC office. He noted that support would still be available for InChI-related projects through the IUPAC Project System.

2.2.3 *Future ACS involvement*

Steve Heller had written back to ACS suggesting a meeting in Washington. It was hoped that this correspondence and the present discussion would result in a fruitful continuing dialogue regarding possible participation in InChI developments.

2.3 InChI Trust office facilities

Ulrich Roessler and René Deplanque reported that the InChI Trust office had been set up at FIZ-Chemie at no cost to the Trust and the website inchi-trust.org had been registered. Ulrich Roessler would be managing the Trust facilities. e-Mail addresses (xxxx@inchi-trust.org) had been established for Board members and it was intended to set up wiki systems for ongoing discussions of working groups. Initial work on the website would concentrate on collecting available InChI information.

Igor Pletnev noted that a previous committee meeting had requested a development server, including facilities for testing InChI implementations; he would discuss precise requirements with Ulrich Roessler and René Deplanque.

3.0 Developer's report

Igor Pletnev reported that, subject to agreement over various questions (specified in his circulated report), the next version of the InChI software would probably be available by mid-October. It would include one bug fix implemented since the release of version 1.02. It was agreed that the new version, which would include both standard and non-standard InChI generation in a single library, would be designated version 1.03. Preparation of a full technical paper on InChI for publication was in progress, and it was hoped to have a draft available by September/October. It was proving difficult to describe the algorithm completely, but it was hoped that a medium-high-level description would be sufficient, in conjunction with the source code. Some reservations were expressed by Kirill Degtyarenko and Dave Martinsen about the lack of a full description, in particular with regard to future portability, and it was agreed that this issue might benefit from further exploration by a contractor. However, John Barnard pointed out the likelihood that even a high-level description would probably not cover all aspects of detail.

3.1 Designation of non-standard InChI

It was agreed that a new (memorising) layer of several characters should be created within the non-standard InChI string to designate the options used in its creation, and that a single letter should be used to designate a non-standard InChIKey. Igor Pletnev would prepare a brief specification for circulation to the subcommittee for comments before implementation.*

3.2 Standard/Non-standard InChI compatibility

It was agreed not to worry about the possibility that a non-standard InChI string may appear identical with a standard string.

3.3 Non-standard InChIKey format

It was agreed that the non-standard InChIKey string should adopt the same format as the standard InChIKey in not containing a check character and using the same proton counting scheme.

3.4 Software release

As noted above, the next software release would be version 1.03 and provide a single package to generate both standard and non-standard forms, specified as 'universal' in the developer's report. However, the already introduced std-InChI API calls should remain, with the code collapsed where possible; Igor Pletnev should feel free to deal with this in whatever way he considered most appropriate.

3.5 Bug fixes and software options

It was agreed that bug fixes and the drawing inconsistency/new normalisation features should be turned on unconditionally. The software options specified in the developer's report were also agreed (subject to the decisions noted in item 3.1). The possibility of introducing annual software releases should be considered seriously.

3.6 Validation test-bed.

It was noted that an InChI/InChIKey validation test bed was required; this would be developed as soon as resource for providing it becomes available.

4.0 Reports from Working Groups

4.1 Resolver

Tony Williams reported that a Google group had been set up to deal with the Resolver discussions. Discussions with National Cancer Institute, RSC and Nature Publishing Group (Tony Hammond) to define a protocol were ongoing. The need for multiple resolvers according to the needs of individual databases was recognised. A draft architecture was currently under discussion, and it was hoped that an example of a functioning resolver protocol would be available by the end of 2009. Sandy Lawson would provide an Elsevier contact for this work, and Chris Steinbeck would be asked whether EBI wished to participate.

* *Secretary's note:* Following subsequent e-mail discussions amongst members of the subcommittee, it has been decided that options memorisation recorded in non-standard InChI will not be retained in the corresponding non-standard InChIKey.

Steve Heller noted that not all organisations with databases will want to set up their own resolvers; we should therefore provide information to users about organisations with resolver facilities that will accept database deposition. The need for a resolver on the Trust website should be considered.

4.2 InChI for Organometallics

The working group proposed that (1) the possibility of carrying out normalisation before metal disconnection be considered; (2) the molfile format be extended to encode more coordination and organometallic structures losslessly. Sandy Lawson agreed to provide details of decisions made for Reaxys.

Igor Pletnev pointed out that implementation of normalisation before disconnection would be a huge job, and it was agreed that it would be preferable to attack the problem initially by developing business rules for structure representation. Further consideration would be needed to (a) define practical options, (b) discuss encoding protocols and (c) look for any convenient ways of modifying disconnection procedures. In Colin Batchelor's absence, Andrey Yerin thought that a further report could be produced by October 1st.

4.3 Business rules for structure input

Andrey Yerin reported that the working group had paid specific attention to stereochemistry, since this area was the most problematic. The need to enforce correct input, with existing IUPAC recommendations as the basis, was clear. It would be desirable to introduce functionality into the InChI algorithm that would warn users of incorrect input, and it was agreed that rules specific to InChI should be extracted from the IUPAC recommendations with this in mind. A status report would be provided by October 1st. Consideration would be given to the possibility of a face-to-face meeting, perhaps alongside the San Francisco ACS meeting.

4.4 InChI for reactions

Preliminary work was proceeding at Cambridge University under the direction of Jonathan Goodman, with funding from RSC. The work was being carried out by summer students, and would continue up to the end of August. A test website allowing conversion from .rxn to RInChI had been established at <http://www-rinchi.ch.cam.ac.uk/>. A project report would be prepared in September for distribution to those Trust members with reaction databases, for comment.

5.0 Future needs

It was envisaged that most of the work of the Subcommittee would be carried out by working groups, and that eventually the Subcommittee would not need to meet more than once a year. The Trust Board would be asked to consider what additional working groups should be established on what timescale. It was noted that stereo-encoding should be added to the list of topics in the Business Plan.

6.0 Next meeting

It was suggested that this take place adjacent to one of the 2010 ACS meetings (March, San Francisco or September, Boston), probably the former.

Alan McNaught
13 August 2009

Appendix C

The following list contains keywords and loosely formulated ideas in almost unedited form as noted by the secretary during the committee's discussion of item 9.8.

- GPM mentioned a radiochemistry meeting to be held by the Royal Society of Chemistry to commemorate Madame Curie's work and the Nobel Prize awarded to her in 1911.
- The American Chemical Society were planning to have postal stamps made.
- KHH suggested the idea of translating Roald Hoffmann's plays into local languages and having them performed in the individual countries.
- The publication of *Principles of Chemical Nomenclature* (cf. item 8.7) could be timed so as to have a release party tied to IYC2011.
- Condensates of parts of *Principles* could be produced for 2011 activities. The 'Essentials of Polymer Nomenclature' proposed by KHH (cf. item 8.9.7) could be an example of such a condensate.
- Tell people how we work in IUPAC.
- Tell people why it is important to use IUPAC nomenclature.
- DStC mentioned that structure representation is important for children learning chemistry. SL said it is important to relate structure to real-life substances, as met with in newspaper articles *etc.* On the other hand, it was also mentioned that there may be an inspirational or entertainment aspect of weird molecules (the 'arsole effect').
- TV programs on chemistry in individual countries.
- Chemistry in old movies (JB).
- Nomenclature games (TD).
- A nomenclature competition.
- Chemistry games (cf. Chemory).
- A chemistry calendar for 2011 (TD).
- An essay competition.
- It was mentioned that CCE (cf. items 13.1 and 14.1) were considering
 - Global experiments related to *e.g.* water quality, climate.
 - Activities to highlight subjects from historical chemistry.
 - A Chemistry Day.
 - A Chemistry Week.
 - Teachers' events.
 - Career fairs.
- In all these efforts, remember that young people are computer-oriented.
- On the other hand, it was stressed that IYC2011 is not only about reaching out to school children.

Appendix D

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

Minutes of the Annual NC-IUBMB and JCBN Nomenclature Meeting Braunschweig, Germany, April 2nd, 2009

Attendees:

NC-IUBMB

Dietmar Schomburg, Chairman (Braunschweig, Germany) Chairman
Minoru Kanehisa (Kyoto, Japan)

NC-IUBMB and JCBN

Keith Tipton (Dublin, Ireland)
Hans Vliegthart (Utrecht, The Netherlands)

JCBN

Gerard Moss (London, UK)
Richard Cammack (London, UK) Treasurer and Secretary

Others

Kristian Axelsen (Copenhagen, Denmark)	Associate member
Ron Caspi (California)	Representative, Metacyc
Karl-Heinz Hellwich (Offenbach, Germany)	Observer
Ida Schomburg, (Braunschweig, Germany)	Observer,
Willy Stalmans (Belgium)	Publications secretary, IUBMB
Edgar Wigender (Göttingen)	Representative of BIOBASE
Wim Vranken (EBI, Cambridge)	Representative of the Protein Databank

1. Welcome and Apologies

Schomburg welcomed the members of the committees, Prof Stalmans and Observers. Apologies were received from Apweiler, Cornish-Bowden, Kuhn and Nicholson.

2. Approval of Agenda

The agenda was approved, with following amendments: Stalmans to give a report under item 5, and Wigender to bring forward his presentation (item 6).

3. Minutes of the Copenhagen Meeting, May 2008

The minutes of the Copenhagen meeting were approved.

4. Matters Arising

Moss reminded the committee of the sad loss of Dr H.B.F. Dixon, one of the founder members of the nomenclature committee, and a long-term contributor of many documents, and enzyme nomenclature. Vliegthart tabled an obituary of Dr Dixon he had written. *Glycoconjugate. J.* 26 (2009) 1. Moss mentioned the obituary in *The Independent* by Simon van Heyningen (<http://www.independent.co.uk/news/obituaries/hal-dixon-cambridge-biochemist-882563.html>)

5. Reports

5.1 Chairman's Report (Schomburg)

The chairman gave an overview on the current projects of JCBN:

12 General guidelines for protein names (document finished)

13 Revision of carbohydrate Nomenclature and Shorter version for biochemists, Missing aspects: e.g. polysaccharides, symbols (under preparation)

14 Small molecules, Nucleic acids, nucleotides, nucleosides, etc. (under preparation)

15 Other protein classes

15.3 Transcription factors

15.4 Peptide Hormones (looking for participants)

16 General biochemical terminology (under preparation)

5.2 Treasurer's Report (Cammack)

Cammack reported that the two IUPAC members had been reimbursed according to IUPAC allowances. The joint NC-IUBMB and JCBN members had been reimbursed, but the titular NC-IUBMB members had not claimed; therefore the committee had remained within budget. In future, titular members should be able to submit their expenses claims to Prof. Jan Joep H. H. M. de Pont (J.dePont@ncmls.ru.nl), send a copy of their claims to Prof Cammack.

5.3 Report from the IUBMB (Stalmans)

The IUBMB had responded to requests that the IUBMB publication Biochemistry and Molecular Biology Education (BAMBED) be made available to members of the Nomenclature committee (NC), and they had been provided electronic access, for two years.

The IUBMB executive was aware of the financial stringency in the NC, and had discussed the possibility of commercial sponsorship of the EC list. Specific enzyme entries might provide links to the product pages of enzyme suppliers. Stalmans proposed such an agreement to the committee. It would be a non-exclusive arrangement, and copyright of the list would remain with IUBMB. After discussion and a vote, it was decided not to proceed with the proposal. The amount of money on offer was small; moreover it was felt that it would prejudice the standing of the NC website as a non-proprietary open source of information.

6. “Classification and nomenclature of Transcription Factors according to their DNA-binding domains”

Wingender made a presentation on the TRANSFAC database of eukaryotic transcription factors, which make up 10% of human genes, and the basis of their classification. It is a hierarchical structure, like the EC list, divided into Level 1: Superclass (general topology; 2: class (functional); 3: family (functional criteria); 4: Subfamily. A public-domain version of the database is freely available for non-profit users.

7. Enzyme Nomenclature and Classification

Schomburg reported on the meeting of the enzyme sub- group, held the previous day,. He provided statistics on numbers added to the list, 1961 – 2009. Enzyme annotation and revision of the list is an ongoing process, and there are probably were several hundred, at various stages of annotation, that needed to be incorporated. (Action – Moss, Schomburg)

Cooperative effort between CAS and NC-IUBMB (Schomburg)

CAS has obtained the detailed enzyme list and in return provided CAS registry numbers to link to individual EC entries.

50th anniversary of the Enzyme List

2011 will see the 50th anniversary of the IUB Report of the Commission on Enzymes, which drew up the EC rules for the Classification and numbering of enzymes. Various possible activities were discussed to celebrate this event, and draw attention to the committee’s activities (Action – All). It would be appropriate to arrange a a special edition of a relevant journal. A number of possible journals were discussed, including the Journal of Biological Chemistry, FEBS Journal, the Biochemical Journal and IUBMB Life. (Action: Schomburg to write to editors).

2011 has been designated the International Year of Chemistry by the United Nations, and national adhering organizations of IUPAC are planning individual events. This might form an appropriate activity for the U.K. (Action: Moss & Schomburg to approach the Royal Society of Chemistry).

8. Future of the Enzyme list (Schomburg, Tipton)

Sinead Boyce, who had much experience of the Enzyme List, had left the enzyme nomenclature group at the end of 2008, owing to the expiry of her funding. The first decision of the Enzyme group was to set up a new Taskforce for enzyme classification, to comprise: Dietmar & Ida Schomburg, Tipton, Moss, Cammack and Caspi. There would also be an advisory group, including Axelsen, Henrissat, Vliegenthart and a representative of KEGG. Further expertise is required in some areas such as enzymes acting on nucleic acids and nucleotides. Other enzyme specialists were discussed, who might be approached (Action: taskforce).

The following procedures were agreed: For each enzyme under consideration, a draft definition will be produced by a member of the taskforce. It will then be circulated for internal review, lasting 1 month; then for public review for a further month. After all comments have been accommodated, the enzyme will be given a new EC number. The person who drafted the entry is responsible for logging all changes made to the definition, and the reasons for them.

The Enzyme sub-group then considered questions about **classification of particular enzymes**, raised by Ida Schomburg and Caspi. Tipton raised the question of reaction mechanisms involving protons, and Cammack of reactions involving light energy (photons). The enzyme sub-group recognized that certain areas were under-represented, such as reactions involving nucleic acids, and complex lipids. Action – all, to look for suitable experts to advise.

A project on Reaction classification was proposed, to incorporate information from the EC list, BRENDA, KEGG and Metacyc. There is partial overlap of databases, but it requires much work to combine them into a comprehensive list. (Action: Schomburg, Tipton, Kanehisa, Caspi).

9 Project on Flavonoid nomenclature

Hellwich tabled a draft application to IUPAC for a project, which was endorsed by the committee. (Action: Hellwich).

10 Recommendations for Terminology, Nomenclature and Databases for Biochemical Thermodynamics

Tipton provided copies of an interim report, which reflected both the chemical and biochemical approaches to the subject. It promised to be a very useful document, as it allowed the calculation of quantities that could not be directly measured by experiment. It was proposed that it should be put on web, and comments to be submitted to Goldberg.

11. Carbohydrate document (Vliegenthart)

Horton had sent comments on a possible future document. This was intended to be an accessible document, to overcome the difficulty that few editors of journals are fully conversant with the correct syntax of carbohydrate nomenclature. Usage is inconsistent in textbooks. The proposed document was intended to be either a list of common examples of compounds with their correct nomenclature, or a set of guidelines to be helpful to biochemists. Hellwich spoke in favour of the aims of the document. Within the next months Vliegenthart will provide a short document (Action: Vliegenthart and Horton to produce a draft document, in consultation with Hellwich).

12. Small molecules glossary (Cammack)

Cammack reported that a draft application had been prepared. Of the previously proposed list of members of the group, Gerard Moss, Marcus Ennis, Susumu Goto, Dietmar Schomburg, Christoph Steinbeck and Gerard Kleywegt as representative of the Protein Databank had agreed to participate, together with a. Karl-Heinz Hellwich also expressed an interest in participating. (Action: Cammack).

Printed version of the Enzyme list (Stalmans, Cammack)

This project is for the IUBMB. The 1992 edition of “Enzyme nomenclature” had been a profitable publication, but was now completely out of date. Cammack had prepared some draft pages for such a book, using information from the ExplorEnz database, and discussed this with Angelo Azzi and a representative of Elsevier. The representative had left the company, and Stalmans had taken responsibility for publications, and so contact needed to be resumed. The size of the list had increased

greatly since putting it on the web, owing to the addition of more alternative names, references, reaction schemes, metabolic maps and other information. For the printed version, this would make the book unwieldy, so issues to be discussed were: which fields to include, and the format of the book. Stalmans would contact Elsevier again to arrange a meeting (Action: Stalmans, Cammack, Tipton).

13. Nomenclature used in PubChem

Tipton reported encountering problems in searching in the PubChem database for common biochemical compounds, such as "glucose-1-phosphate". Some compounds were not named in a way that enabled searching, others were present in numerous copies. This appeared to be a consequence of the automated way in which data are collected from the literature. There is no way of submitting corrections and changing entries. Although it is a very large and potentially useful resource, its value at present is limited. (Action: note taken)

14. Items for Discussion

All items are covered elsewhere in the minutes.

15. Update on Action items from previous years

Update on the phosphorus document (Moss)

(Action: Moss to finalize phosphorus document and submit it to IUPAC).

Letter for distribution to PDB staff on what is needed to classify a new enzyme (Action: Boyce)

Tipton had circulated the "frequently-asked questions" on Enzyme classification, with answers, which accompany the ExplorEnz database. Guidelines on the submission of new enzyme entries is already on the website under "Advice".

Tipton suggested that the committee should consider updating many of the items in the "White Book"

Tipton reiterated that this would be a useful activity.

16. Funding situation and possibilities (Schomburg)

Schomburg reported that he had send a grant proposal to Beilstein to fund the development of the enzyme list. Despite positive scientific evaluation it was not funded because the contract between Beilstein and Elsevier precluded their being used to support database activities for 2 - 6 years.

EU, NSF, and NIH funding were being investigated.

Vranken mentioned that the Wellcome Trust had funds for database work.

17. Election of new secretary

Following the resignation of Boyce, Cammack agreed to stand for election as Secretary. He was elected *nem con* in a ballot of titular members.

18 Membership of Committees

Schomburg introduced the revisions to the list of members. He recommended that where members were listed on the website, the projects for which they were responsible should be provided, as well as their positions on the committee.

Cammack agreed to act as Secretary for a year, and continue to act as Treasurer. He would prepare the minutes and agenda for next year, and act as the contact point for the committee in place of Boyce. . A new secretary would be sought for 2010 onwards (Action: Schomburg)

McNaught had resigned from some of his nomenclature activities. Moss would ask him if he would remain available to respond to questions in his areas of expertise. (Action Moss)

Cornish-Bowden had not attended meetings for some years. Tipton and Hellwich undertook to consider changes to the Kinetics document and forward comments to him (Action: Tipton and Hellwich).

New Associate members: Ida Schomburg and Kristian Axelsson

Retired from the list: Alan Chester, Toni Kazic, Associate members of JCBN, were to be thanked for contributions, in the hope that they could still be contacted for questions within their expertise (Action – Schomburg)

19. Any Other Business

The committee was saddened to hear of the death of Ed Wood, the editor of BAMBED, and an enthusiastic supporter of Nicholson's metabolic maps and activities. Tipton reported that Nicholson continued to be very active, and planned to attend the Cambridge meeting. His website, containing Animaps, was receiving hundreds of hits per day.

20. Date and Place of Meeting in 2010

Possibilities were Cambridge (Franken), Boston (Kanehisa) or Utrecht (Vliegenthart). A vote was in favour of Cambridge 2010 Apr 16 – 18th. There could be satellite meetings of the enzymes group, small molecules group, and any other projects at that time approved.

21. Open Forum

No further issues were raised that were not already in the agenda.

Appendix E

Report from Division II (Jan Reedijk; August 1, 2009) for ICTNS and Division VIII

- a) element 112 name and its abbreviation
- b) element 74: tungsten name(s)

About element 112: The early (and bad) publicity on Cp and Copernicium is regretted.

The division can agree with the proposed name for the element; the proposed symbol, however, is not accepted, for 2 main reasons, namely: The symbol Cp is a most common and frequently used ligand abbreviation. Moreover, the abbreviation Cp was once proposed and used (and rejected by IUPAC). An IUPAC decision from 2002 was that once rejected, a symbol (or name) cannot be proposed for another element. (W.H. Koppenol, *Pure Appl. Chem.*, **74**, 787–791, 2002). This will be communicated to the proposer using the official route. *N.B.* The Division has discussed possible alternative abbreviations, but is not allowed to make suggestions for alternatives to the proposers.

About a possible allowed second name for element 74, W:

Division II had asked division VIII to reconsider their earlier decision (2005 Red Book) on one or two names for W. The 2008 motion was: “*Division II recommends that Division VIII consider going back to the designation tungsten (wolfram) for element #74, that was used in the 1990 edition of the Red Book*”

This item has been discussed in detail by Division VIII (July 31, 2009), and the outcome was evaluated in Division II on August 1. It was concluded and agreed that:

1. The 2005 paper in *Chem. International* (Damhus et al.) is still valid in its entirety.
2. The text in the old Red Book was primarily meant as a service to the reader that also “Wolfram” occurs; (but in documents on polyoxometallates CNIC was not always so clear in the past)
3. The 6-page 2008 memo on the history of naming elements written by Norman Holden was well received and highly agreed with.
4. No new convincing arguments in favour of allowing also wolfram were presented.
5. As before, in other languages one is free to use names based on wolfram; (like for K, Na, Hg...)

Additional comments:

6. The accepted PIN system (Preferred IUPAC Names for compounds) would NOT allow a name for W different from tungsten.
7. The use of wolfram in Mexico appears as not occurring.
8. The use of wolfram(ate) in and outside of Spain is also very limited, as shown from a July 31, 2009 search on Web Of Science (covering papers from the period 2000-2009): Only 1 paper written in English was found using wolfram(ate) in title, abstract or keywords.

Details:

Tungsten or tungstate: yields 19416 hits (2000-2009)

Wolfram or wolfram(ate): yields 598 hits (most of which are NOT chemistry, and deal with medicinal aspects, like “wolfram syndrome”), or have “Wolfram” as part of a person’s name in the text.

Wolfram or wolfram(ate) (and a Spanish address): yields only **21 hits** (from which only 3 are about chemistry: 2 from a journal written in Spanish, *Revista de Metallurgia*; only one paper was in English: *Journal of Physical Chemistry A* **111** (2007), 9969-9977 *Mixed-valence polyoxometalates: Spin-coupling and electron distribution in the decawolfram(ate) anion reduced by two electrons*).

[Secretary's remark to the report: Item 6 under element 74 speaks of 'the accepted PIN system (preferred IUPAC names for compounds)'. There is no accepted *system* at this time, in fact even no PINs, strictly speaking. Once we *do* get the PINs, they will have to comprise also names derived from element names such as tungstide and tungsten(6+), so it is not only *compound* names.]