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

Minutes of Division Committee meeting

Büdingen, Germany, 31 July–1 August 2008

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

Associate Members
Jaroslav Kahovec (Czech Republic) **JK**
Alexander Lawson (Germany) **SL** (only part-time)
József Nyitrai (Hungary) **JN**
Warren H. Powell (United States) **WHP**
Andrey Yerin (Russia) **AY**

Observers
Bernardo Herold (secretary, ICTNS; Portugal) **BH**
Hervé Schepers (European Commission; Belgium) **HS**
Jiři Vohlídal (Czech Republic) **JV** (only part-time)

The complete Division VIII Committee membership is given in Appendix A.

1. Introductory remarks and housekeeping announcements.

GPM welcomed the Division Committee and the observers.
He also thanked KHH for taking care of all the practical arrangements in connection with the meeting in Büdingen.
KHH mentioned that the refreshments for the coffee breaks throughout the week had been sponsored by the company Evonik Degussa, and that the tour to Ronneburg (a social event to take place in the evening) was sponsored by Springer-Verlag. KHH explained that his book in German on stereochemistry had been published by Springer and that his latest books were on display in the meeting room.

2. Apologies for absence.

Apologies had been received from the following Division Committee members who were not able to participate: Farzana Latif Ansari (had not been able to raise funding for travelling), Ebbe Nordlander, Hiroshi Ogino and Jan Reedijk. Michael Booth, secretary of Committee on Chemistry and Industry (COCI), had also been invited, but had not been able to participate.

During the meeting a message was given by GPM that JCBN member Hal Dixon had passed away a few days earlier. Regrets were sent on behalf of the committee.

3. Introduction of attendees.

A quick round of introductions around the table was made.

4. Approval of agenda.

The agenda was approved with the remark from GPM that certain items would have to be dealt with out of order because some attendees would not be present during the entire meeting. [TD comment: the agenda items are minuted here in the order of the agenda as originally distributed, *i.e.* not chronologically.]

5. Minutes of meeting in Turin 4-5 August 2007 (prepared by WHP).

The minutes were approved with a few minor corrections. Also, it was agreed that KHH would send a further few trivial corrections to TD soon after the meeting, after which the minutes would be considered completed and ready for posting on the Division VIII webboard. [TD comment: at the time of writing these minutes, the Turin minutes in their final form have been posted on the Division VIII webboard, and the secretariat has been inquired about posting them on the IUPAC website.]

6. Matters arising.

The schedule for the meeting was summarised.

7. Publications since the 2007 meeting.

7.1 Representation of configuration in coordination polyhedra and the extension of current methodology to coordination numbers greater than six (IUPAC Technical Report), R. M. Hartshorn, E. Hey-Hawkins, R. Kalio, and G. Jeffery Leigh, *Pure Appl. Chem.* **79**(10) 1779-1799 (2007); doi:10.1351/ pac200779101779

7.2 Structure-based nomenclature for cyclic organic macromolecules (IUPAC Recommendations 2008), W. Mormann and K.-H. Hellwich, *Pure Appl. Chem.* **80**(2) 201-232 (2008); doi:10.1351/ pac200880020201

7.3 Graphical representation standards for chemical structure diagrams (IUPAC Recommendations 2008), J. Brecher, *Pure Appl. Chem.* **80**(2) 277-410 (2008); doi:10.1351/pac200880020277

7.4 Corrections to *Red Book* 2005 [see www.chem.qmul.ac.uk/iupac/bibliog/RBcorrect.html**]**

KHH and JB had received reprints of the cyclic macromolecules paper (7.2) and the graphical representation paper (7.3), respectively. These reprints were available at the meeting.

KHH mentioned that his book *Stereochemie – Grundbegriffe* (Stereochemistry – Basic concepts) had appeared in 2007 in its 2nd edition (from Springer-Verlag). An English translation was planned, but will not appear within the next year.
Furthermore, the 3rd edition of KHH's nomenclature book was due to appear in October 2008. New features in it would include changes made in the 2005 Red Book and the naming of racemates.

See also minute **13.1**, translations.

8. Division VIII projects.

8.1 The IUPAC International Chemical Identifier (InChI) (2007-052-1-800) (SRH).

8.1.1 Status.

Since Turin, SRH had had quite a number of contacts and had given several talks about the InChI. He reported that the InChI has now been widely adopted by databases (*e.g.* Beilstein, EBI) and publishers (*e.g.* RSC). Microsoft is expected to integrate it and vendors of structure drawing software will be approached. Artus Labs, a small company in North Carolina, had indicated an interest in creating a 3D InChI and was to be approached.
Version 1.0.2 of the InChI was to be launched later in 2008; anyone interested in an electronic version should approach SRH.
For further details, see SRH's report on the InChI project, added here as Appendix B.

8.1.2 Project proposal for Reaction Identifiers.
SRH reported from a meeting held in Berlin in May 2008 about developing a mark-up language equivalent of the InChI for chemical reactions. The first phase of the work, estimated at 9 months' duration, had begun recently with a student (Colin Batchelor) funded at RSC. Resources had yet to be found for a second phase estimated at 2 years.
Minutes by SRH from the Berlin meeting are included here as Appendix C. This project is to be seen as complementary to the prospective project on standards for graphical representation of reactions (minute 9.1). The two projects should agree, of course, on the contents that need to be displayed.

8.1.3 Funding of InChI development in the future (support for Igor Pletnev).
A lengthy discussion ensued about how to secure future maintenance of the InChI. SRH's Division VIII term ends in 2009 and a stable, long-term agreement should be sought for. The IUPAC secretariat, CPEP and Division VIII were all seen as bodies within IUPAC that should feel some responsibility for maintaining the code and also for continuing efforts towards publicizing the InChI. However, the IUPAC project system was not seen as the most appropriate instrument for this.
The outcome was that Division VIII will set up a subcommittee (not necessarily a subset of the Division Committee) to oversee maintenance, publicity and initiatives on extensions of the InChI (such as into polymers, Markush structures, chemical reactions). A tentative manning of the subcommittee could be SRH (chair), AY, SL, Alan McNaught, A. (Tony) Williams (ChemSpider), E. Bolton (National Institutes of Health). Further places to recruit members could be National Cancer Institute, PubChem/National Center for Biotechnology Information, Royal Society of Chemistry, Wiley, Elsevier, CAS, ACS, Microsoft and other organisations. JB was offered membership, but declined. JW was asked to check with Chemical Abtracts what their interest might be. Still others should probably be approached.
GPM was to initiate the formation of the subcommittee and see to it that it got started soon and was also to contact CPEP about these plans.
Igor Pletnev must now write a report on the status of the InChI project, even if there are still bugs that one would like to fix. The report should go to PAC and the goal should be that it documents the code, but is readable to a non-progammer. (AY to talk to Pletnev in Moscow.)

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

8.2.1 Overall status.
Last year Chapters 2, 3, 9, and 10 were noted as being complete. In the past year the team had worked at Chapters 1, 4, and 5. Chapter 4 had been expanded, Section P-47 still needed to be completed. Chapter 6 was being worked in bits; after a complete reworking of P-63, sections P-60 to P-63 were more or less ready for review, while P-65 was still being worked at.
Chapter 7 was coming along, while Henri Favre was to go through Chapter 8 now. Appendix I was ready; Appendices II and III needed a bit more work. The latter will be a list connecting the 1979 Blue Book to the new one.
Preselected names only will be given for substituent groups, but ions and radicals will get PINs.
Chapters 1,2,3 are pretty much ready for review.

Some outstanding issues in the individual chapters were highlighted:

- fitting symbols such as '[' and '{ ' into the alphanumerical order established for letters and numbers (which already includes locants such as *N′*, *N″*)
- in Chapter 5 (which summarises all the cases from chapters 1–4 where a choice needs to be made) there are still problems with some fullerene derivatives – should they be named on the basis of fused rings or parent fullerenes, how to use 'nor', how many bonds may be cut in a fullerene structure before the name is to be built on substructures instead etc. – thus the wording

is only preliminary.

This entailed some discussion about whether there are limits to our procedures for assigning P-names (or to our knowledge about such limits...). It was noted that section F puts restrictions on the numbers of modifiers used in a name for natural product.

All in all, based on the progress made, WHP anticipated that the entire book would be ready for posting on the webboard in April 2009. WHP will send an overview of the situation.

8.2.2 Dividing line between additive and substitutive nomenclature.
More precisely, the discussion was about exactly where to draw the line between the areas of responsibility of the organic and inorganic PINs group, respectively, when it comes to the assignment of PINs to compounds containing carbon as well as one or more elements from the lower parts of groups 13 to 16. This will have consequences for exactly which of such compounds will be given a PIN in the upcoming Blue Book. A proposal for this was made by RMH on the basis of work in the inorganic PINs group prior to the Division Committee meeting. However, the discussion was difficult to separate from the discusssion of which naming principles should be followed by whichever group was to assign the PINs. A main point made was that IUPAC should follow CAS whenever there was no good reason to deviate. Subsequent to the meeting, E-mail discussions revealed that there was not agreement on what the consequences of this policy would be, in part because an extract of the relevant CAS rules had not been available at the meeting in a form appropriate for everyone to appreciate these rules. The issue has not been resolved at the time of completing these minutes.

8.2.3 Anion names.
a. Names needed for ligand parts of PINs of coordination compounds.
The generic example of a problem anion for which a name is needed in order to form the corresponding ligand prefix is acetylacetonate, which systematically can be named either 2,4-dioxopentan-3-ide or 4-oxopent-2-en-2-olate, according to which hydronated form is chosen as the parent forming the basis for the name construction. A rule is clearly needed to make that choice. WHP promised that the Blue Book will contain such a rule (a proposal for such a rule had been worked out at the Blue Book meeting the day before). If one further wishes to indicate the delocalisation, a descriptor 'deloc' may be applied; JW said that CAS does this, but WHP said it is not going to be introduced in the Blue Book.
b. Request from the ionic liquids community (TD).
Cf. earlier correspondence with G.J. Wilson, and the article: G.J. Wilson, A.F. Hollenkamp, A.G. Pandolfo: Resolving Ambiguous Naming for an Ionic Liquid Anion, *Chemistry International* **29** (4), July-August 2007. This was about naming anions formed by loss of a hydron from a nitrogen further carrying two substituted alkylsulfonyl groups (various names ending in 'ide' have been used in the literature).
Again, the Blue Book team would make sure that the upcoming rules provide for naming such anions.

8.3 Nomenclature for rotaxanes and pseudorotaxanes (2002-007-1-800) (AY).
A status report was given by AY. [TD: A written report was posted on the Division VIII webboard soon after Büdingen and is included here, lightly edited, as appendix D.]
The recommendations resulting from what AY now called the first part of the project (no consideration of stereoisomerism) had been accepted for publication in PAC [TD: and have been published since the Büdingen meeting: *Pure Appl. Chem*. **80**(9), 2041-2068, 2008].
Stereoisomerism of rotaxanes had turned out to present some fundamental problems for nomenclature and terminology. These are discussed in Appendix E of these minutes. AY had convened a small meeting the day before the Division Committee meeting that had addressed these problems. The presentations given at that meeting will be subsequently posted on the Division VIII web board [TD: this has happened]. The

discussion had brought forth some suggestions for the description of symmetry properties of rotaxane components, in particular in BH's presentation, but no firm decisions were made.
RMH urged the group to also make appropriate use of point groups in the description of particularly chiral systems.

8.4 Cyclic peptides (2004-024-1-800) (GPM).
No news to report.

8.5 Nomenclature of phosphorus-containing compounds of biochemical importance (2006-019-1-800) (GPM).
To be posted on the webboard.

8.6 Comparison of procedures for naming hydro derivatives of fused ring systems (WHP).
It was discussed whether the document is properly classified as a technical report or a recommendation. WHP will submit it as a recommendation.

8.7 Second edition of *Principles of Chemical Nomenclature, A Guide to IUPAC Recommendations* (2006-029-1-800) (GJL).
The Principles group had held a meeting the day before the Division Committee meeting. GJL reported that the project plan had largely worked in that about 90 % of the material was in, but said there were differences of opinion regarding the style of the book: expositionary or rule by rule. In the last end, the editor will have to make the choice.
The production plan will have to be prolonged a bit. Currently it is the intention that all authors complete their part by the end of November, and a grand editorial meeting is then to be held at around Easter 2009.
Deciphering of names will be part of the book.
A publisher has not yet been chosen.
GPM said the book should go on the webboard for discussion. [TD remark: Some chapters have now been posted.]

8.8 Preferred names for inorganic compounds (2006-038-1-800) (RMH).
The inorganic PINs (preferred IUPAC names) group had met in the days before the Division VIII meeting, both separately and together with the organic PINs (Blue Book) team. The main issues dealt with had been:

- The idea of having several levels of PINs according to the degree of detail one wants to communicate with the PINs, including whether there should be a fixed or variable number of levels of PINs for various classes of compounds. Also the idea of letting PINs somehow carry a date, similarly to CAS stating that a name is a '9th collective index name'.
  Having different levels of PINs may in fact ease the communication in technical and less scientific settings.
  TD suggested to let the PINs levels match the InChI levels, but JB remarked that there are already problems with the InChI levels (to be discussed further with SRH).

- The choice of central atoms to be used in additive names of the coordination type.

- The use of an extended kappa system to enable the specification of ligating atoms in ligands the names of which are themselves coordination-type additive names.

- Defining the borderline beween organic and inorganic PINs when it comes to organometallic compounds (see minute 8.2.2).

It was remarked that the criterion that a name is sufficently elaborate if it is not ambiguous, will not

be valid in the future where a computer has to be able to work out the structure from a name; 'not ambiguous' is not a computerisable concept.

RMH summarised some main hurdles that still lay ahead:

- Delocalised anions as ligands (cf. minute 8.2.3).
- More work on κ, η, and μ, including the 'κ_L device' used for distinguishing kappas referring to ligation to central atoms within a ligand or on a higher level within a coordination complex containing that ligand. In principle, μ is superfluous, but nevertheless it is planned to include it in PINs for clarity.
- When to use rings and chains – a decision tree is being worked out.
- Preparing a list of retained names.

HS (cf. minute 15) agreed to join the PINs group.

8.9 Macromolecular projects (with Division IV).
JK, KHH and PH had recently participated in a meeting in Taipei of the Division IV Subcommittee on Polymer Terminology, of which they are all members. The minutes from that meeting were not yet available.

8.9.1 Source-based nomenclature of single-strand organic polymers (2003-042-1-800) (PH).
This ongoing project had been extended to encompass also double-strand polymers and copolymers, and generic source-based nomenclature was also to be included, but only with two examples explaining the principle and a reference to the separate document [*Pure Appl. Chem.* **73**(9), 1511-1519 (2001)].

8.9.2 Nomenclature for chemically modified polymers (1999-051-1-800) (PH).
The project document was now in a fairly advanced state. Prof. T. Kitayama was to transfer it shortly to PH for a check of the English.

8.9.3 Nomenclature for rotaxane polymers (2007-009-1-800) (JV, AY).
This project had been taken over by JV from Ted Wilks and had been waiting for the rotaxanes document (from project 2002-007-1-800, cf. minute 8.3). In the meantime, JV and AY had revised and shortened the project document. Working group members had provided feedback, and the document was mostly in the polishing stage, however with issues remaining in the overlap area between nomenclature for regular polymers and the new recommendations.
An open question is how to post this type of interdivisional document on the webboard.
[TD remark: it is being investigated how a joint webboard for several divisions can be set up.]

8.9.4 Terminology and structure-based nomenclature of dendritic and hyperbranched polymers (2001-081-1-800) (JK).
The document was now arranged in two parts, one on dendrimers and one on hyperbranched polymers, respectively, the latest versions of which dated to April 14, 2008. KHH had made substantial comments in June 2008 on the version he had received then, dated May 2007, and JK will amend the documents taking these into consideration. Additional input from Division VIII would be helpful. Next, the documents should go on the Division VIII webboard and, concurrently, for public review. (The draft was on the webboard last year.)

8.9.5 Glossary of class names of polymers based on their chemical structure and molecular architecture (2002-014-1-400) (JV).
Comments had been called for on the (old) IUPAC website with a deadline on June 30, 2008. The document was still available for download there. KHH had corrections that he would send to JV by

August 15 [TD/KHH: this happened later for about half of the document and early in 2009 for the rest of the document].

8.9.6 Preferred names for polymers – list of preferred, acceptable (other IUPAC-approved) and not acceptable (wrong or outdated) names for polymers (2008-015-1-400) (KHH).
The intention was to produce a table-like database of constitutional repeating units and common polymers with specification and classification as preferred, acceptable, not acceptable (outdated, ambiguous, wrong) for each name (ever) used for them in any IUPAC document.

8.10 Other interdivisional projects.

8.10.1 Classification, terminology and nomenclature of borophosphates (2003-034-1-200) (with Div.II)**.**
There was no news.

8.10.2 Recommendations for nomenclature and databases for biochemical thermodynamics (2006-023-3-100).
This document is held up by ICTNS which is insisting on strict IUPAC style for an audience of biochemists. This is unacceptable to the biochemists. It is to be hoped this can be resolved by adding a note of where the two groups of workers have different conventions.

9. Future projects.

9.1 Graphical representation of reactions.
No news. In Turin, Danielle Gibney had been interested and had contributed to a scoping exercise organised by Bill Town. A project needs to be set up and Bill Town should be approached.

9.2 Revision of IUPAC web document *Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology* (PH).
PH had prepared a project proposal.
[TD: The project has since been successful and it started formally on August 1, 2008 (2008-020-1-400).]

9.3 Essentials of polymer nomenclature (KHH).
The intention is to create a two-page pocket guide for students and journals in hardcopy as well as web format. [Project proposal submitted in September 2008 and accepted later in 2008.]

9.4 Stereochemical notation in polymers (KHH).
The background is that there is inconsistent terminology in the area. D. Jones had asked KHH to write a project proposal and this will happen sometime later this year – the submission date had not yet been fixed.

9.5 Graphical representation of polymers (JK, KHH).
The existing document [Graphic Representations (Chemical Formulae) of Macromolecules (IUPAC Recommendations 1994), *Pure Appl. Chem.* **66**, 2469-2482 (1994)] needs updating. This is not yet in the works.

9.6 Metallacycles (ATH, WHP).
No progress to report.

9.7 Boron nomenclature.
No progress to report. WHP remarked that P-68 of the new Blue Book will have some treatment of organic boron compounds.

9.8 Other projects.
Terminology at large and in particular in the Gold Book (GB) were discussed. BH explained that there is no current project specifically focusing on adding terms or revising terms in GB.

A document had been circulated from ICTNS to the Divisions in late July 2007. It contained (examples of) questionable or obviously erroneous entries in GB. One such obvious example was the explanation of the Haworth representation of cyclic forms of monosaccharides, in which a drawing of a glucofuranose structure was labeled 'glucopyranose'. For more intricate definitions, such as that for 'molecule', where there is apparently disagreement in the community on the desirable content of the definition (are monoatomic species allowed or not), the division responsible for the term must take over the case.
[TD remark: the Haworth explanation has in the meantime been corrected in the online GB. The 'about' page there gives the history of GB since the printed second version in 1997 and states that 'new content and features are added as part of IUPAC project 'Enhancement of the electronic version of the IUPAC Compendium of Chemical Terminology'.]

KHH remarked that it might be worthwhile considering preparing an 'essentials' version of GB (cf. minute 9.3).

TD reported about a Danish pilot study that had been presented at the JCBN meeting in Copenhagen in May 2007 (cf. minute 14.6). A group consisting of a biochemist emeritus, two professional terminologists and TD are having a look at a more narrow subject, in principle arbitrarily chosen, namely terminology in enzyme chemistry. The group will work a bit more before considering proposing a formal IUPAC-IUBMB project. KD volunteered to participate in the project.

JW is involved as a CAS representative with an ISO group dealing officially with 'nomenclature of nanotechnology' (should probably rather be called terminology). It was discussed whether Division VIII as such should be involved. RMH remarked that there are clusters in nanoscience the nomenclature of which could be a subject appropriately dealt with in Division VIII. JW will keep RMH informed about these activities.

10. Should IUPAC endorse particular formats of the Periodic Table? (GJL).
GJL told that he is approached every so often by people who are interested in the periodic table and who suggest alternative layouts to the so-called IUPAC version in the Red Book and seek IUPAC endorsement of their variants. Four pages were circulated that displayed one such alternative. Also, by way of exemplifying the continuing interest in layouts of the periodic table, KHH had circulated before the meeting the paper "The Role of Triads in the Evolution of the Periodic Table: Past and Present" by E. Scerri, *J.Chem. Educ.*, and furthermore former CNIC chairman Herb Kaesz' article with Peter Atkins "A Central Position for Hydrogen in the Periodic Table " [*Chemistry International* **25**(6), 2003] was mentioned [TD note: see also comments inspired by the latter article in *CI* **26**(3), 2004]. Following a brief discussion, it was decided that GJL would draft an article for CI on the subject. [TD remark: the article has appeared since; see G.J. Leigh: Periodic Tables and IUPAC, *Chemistry International* **31**(1), 4-6 (2009).]

11. Membership.

11.1 Election procedures.
11.2 Committee membership, titular and associate members (current membership, see Appendix). Tony Williams suggested to replace SRH.
11.3 Nominating committee to select candidates for titular members 2010-2011.

The procedures for election for division membership 2010-11 had been described in an E-mail dated May 3, 2008, from GPM to the Division Committee:

> There will not be elections at the 2009 General Assembly, because the elections have to be over before the Bureau meeting planned for a few months in advance of the GA. [TD remark: the Bureau meeting has been fixed in the meantime to take place April 18-19, 2009].
> The officers for 2010-11 were assumed to follow normal practice in that GPM was to become Past-President and RMH to become President. TD was willing to continue as secretary.
> SRH and KHH had completed their four years as titular members.

In the meantime a nominating committe for candidates for the single vacancy for a new titular member of the Division Committee had been formed:
Jim Bull (chairman), RMH, Alan McNaught, Michael Hess and Lenn Lindoy (University of Sydney, Australia).

Nothing else had happened yet.

11.4 Advisory subcommittee 2008-.
Nominations shold be sent to GPM. It was agreed that there should be a specific webboard for the Advisory Subcommittee. GPM agreed to take care of this.

12. Webboard.

SRH said the secretariat had noticed very low usage of the Division VIII webboard and several attendees reported problems in accessing the webboard. [TD: These problems were solved shortly after the meeting, however, through efforts by the FIZ-Chemie team in Berlin.]
Outstanding issues were to establish a separate webboard for the Advisory Subcommittee, most probably including all Division VIII members as well, and to retrieve the material from the old RSC-hosted Division VIII webboard.

13. Publicity.

13.1 Translations.
The Red Book had been translated into Spanish:

M.A. Ciriano and P.R. Polo: *Nomenclatura de Química Inorgánica, Recomendaciones de la IUPAC de 2005,* Prensas Universitarias de Zaragoza, 2007 [ISBN 978-84-7733-905-2]

and into Hungarian:

P. Fodor-Csányi, Gy. Horányi, T. Kiss and L. Simándi, *Szervetlen kémiai nevezéktan, a IUPAC 2005, évi szabályai,* Akadémiai Kiadó, Budapest, 2008, 407 pp [ISBN 978-963-05-8559-0].

BH told that there is a team in Portugal translating the Red Book, and that a Brazilian-Portuguese translation of the carbohydrate document [Nomenclature of Carbohydrates (Recommendations 1996), *Pure Appl. Chem.* **68**, 919-2008 (1996)] was being prepared. BH to send E-mail with information.

KHH's books in German on nomenclature and stereochemical concepts (see minute 7) are based on IUPAC rules, but no German translations of IUPAC rules *per se* were planned.

Bibliographical information on translations may be retrieved in general at
http://www.chem.qmul.ac.uk/iupac/bibliog/

13.2 IUPAC and IUBMB nomenclature web site (GPM).
GPM said it was too early to assess the activity on this site in 2008. A table from May 12, 2008 giving figures for average use per week (specified for the various documents available on the web site) was passed around. See http://www.chem.qmul.ac.uk/iupac/usage/summary.html

13.3 IUPAC website (SRH).
The new website is currently hosted by FIZ Chemie in Berlin. The German Chemical Society has committed to ensuring maintenance, although the problem was noted that there is no firm structure for administration of the website within IUPAC and no goals or milestones have been set up. In principle, Fabienne Meyers was believed to be responsible for this.
The software group in Prague was commended for its good technical work. Nevertheless, the comment has been made that the website seems more focused towards IUPAC members than chemists at large. Also, there are still problems for some users in that their browsers do not open the new webpages properly and they do not get access to all the functions there. Furthermore, there are no URL's, and Google does not find the files that only generate HTML 'on the fly'.
There seems to be no concrete plan for the old website. GPM will contact Fabienne Meyers/the secretariat and/or CPEP about eventually removing it.

14. Reports from other bodies.

14.1 Committee on Chemistry Education (CCE) (RMH).
RMH reported that the CCE had met in Turin just after the 2007 Division VIII meeting and again was to meet just after the Büdingen meeting. The project to have 2011 as the Year of Chemistry had been approved by the UNESCO board and now was on its way in the UNESCO bureaucracy. [TD remark: on December 30, 2008, the UN has declared 2011 the Year of Chemistry. The story is on www.iupac.org.] .
Division VIII should now consider what to do for 2011. GPM said the Divison presidents need to get information from CCE. KHH remarked that the 'essentials' publications (see minute 9.3) could be relevant.

14.2 Committee on Printed and Electronic Publications (CPEP) (SRH).
CPEP had also discussed the IUPAC website (see minute 13.3 and Appendix B).
All of PAC is now online and available. Anyone can get the back issues for free on the IUPAC website, but access to the current year is via subscription only. *And* subscribers must go through a subscription agency – not the IUPAC website.
An IUPAC project proposal to "InChIfy" PAC has been submitted to IUPAC for funding and SRH assumed this would materialise already this year. (See Appendix B.) The exact scope of this was not entirely clear, *e.g.* to what extent would manual curating be necessary. Apparently it is not trivial to go from the structural diagrams in PAC to a format that will allow for generation af the InChI. JB asked whether CAS might help by providing the structures they extracted from PAC. JW replied by referring to the SureChem portal [provided by ReelTwo and ACDLabs, http://www.reeltwo.com], a facility offering to scan *e.g.* patent literature for chemical structures.
SRH asked on behalf of CPEP whether the new Blue Book will contain InChI's. GPM replied that we do not know at this time, but it is in any case not relevant for the printed version of the book.

14.3 Committee on Chemistry and Industry (COCI) (GPM).
Nothing to report. The minutes of the 2008 annual meeting of COCI had been circulated [TD remark: they are now available on the web].

14.4 PAC Editorial Board (GPM).
The editorial board only meets every second year, so there was no report. Jim Bull, editor-in-chief of PAC, had stated that the ISI rating for PAC had doubled in the last five years.

BH noted that the technical reports and recommendations are seldom quoted and asked whether it would be possible to register the number of hits for these document types.
It was further mentioned that the citation style of references had been changed: article titles and page ranges are no longer accepted (only the first page of a publication). This was a (questionable) decision of the editorial board.

14.5 Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS) (JN).
JN had noting to report. The last meeting had been in Turin in 2007.

14.6 Report of JCBN meeting in Copenhagen 16-17 May 2008 (GPM, TD).
The minutes (not yet formally approved) as received from the JCBN secretary date from September 2008. They are included here as Appendix F.
The carbohydrates document needs updating, and in particular the disaccharides and polysaccharides sections need to be expanded.
A newsletter from JCBN will hopefully soon appear.

15. Any other business.

The Division Committee heard a 42-slide presentation entitled *Customs and IUPAC–Traceability of Chemicals in the Customs Jungle* given by observer HS from the European Commission. [TD remark: this presentation has since been made available on the Division VIII webboard.]

The presentation dealt with the European Union customs system including the GCL (Group of European Customs Laboratories, 81 in all in the various Member States) and the large number of databases the system is based on, including the ECICS (European Customs Inventory of Chemical Substances). The purpose of the customs system is to be able to control traffic for the benefit of budget, trade, health and environment in the Member States, the combat of terrorism, *etc.*

The presentation described in all 8 'jungles' in the customs world: chemicals, names, numbers and identifiers, databases, *etc.*

The ECICS, which is used world-wide, since the 1970s features a translation module for IUPAC names and uses a number of other identifers as well, such as INN and ISO names. It is freely accessible at http://ec.europa.eu/taxation_customs/dds/ecicau_en.htm.

A number of projects associated with the ECICS and planned to culminate in the next few years aim at improving translations and supplementing and checking nomenclature.
IUPAC nomenclature is one of the cornerstones of the databases, but customs also needs trivial and semi-systematic names and short designations like the INN and the ISO names.

HS advertised a conference, ECICS-2, to take place in 2009, and the 4th Conference of European Customs Chemists in 2010.

HS is interested in IUPAC's help to check the translations of summary lists, the glossary and the rules of the translation module needed for the automatisation of translations. In return, HS can provide to IUPAC:

> The summary list of IUPAC chemicals names in all European languages.
> The publication on the TAXUD DDS website of PINs and other IUPAC names (accepted, obsolete, ...).
> Advertisements for the *Blue Book, Principles, etc.*, internally in the customs system.

The presentation ended with a 'IUPAC conclusion':

> Customs need clarity, certainty, simplicity and especially stability – evolution is preferable to revolution.
> Do not kill trivial and short names!
> Customs need a maximum of PINs in all domains.
> Customs appreciate IUPAC's work very much.

GPM finally remarked thay COCI ought to be involved in IUPAC's contact to the European Commission.

16. Date and time of next meeting.

Glasgow, UK, July-August 2009. More precisely, Division VIII Committee meeting presumably July 31 to August 1, with working group meetings in the days immediately before. The inorganic PINs group anticipated the need for a two days' meeting. There might also be a need for a *Principles* meeting.

Appendix A
Division VIII Committee, membership as of July 2008

Gerard P. Moss (United Kingdom)
President
Richard Hartshorn (New Zealand)
Vice President
Ture Damhus (Denmark)
Secrectary

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

InChI Status Report
July 2008 – Stephen Heller

At a recent BioIT conference, when asked about how he decided an IT/computer project was working well, the CEO of Vertex Pharmaceuticals made the remark that he considered it a success and defined success as "uncoerced adoption". This is exactly the right time for the IUPAC InChI.

Acceptance and usage of InChI has progressed much more rapidly than one could have optimistically hoped for. Every large database of chemical structures associated with chemical data (I exclude the CAS database as it is associated with the chemical literature) has incorporated InChI. These large database files range from about 36 million structures (larger than the CA database) to some 2-3 million. In addition there are dozens of databases with a few hundred to a few thousand chemical structures that have added InChI to their file records. One recent database to incorporate InChI is the Beilstein database, now owned by Elsevier.

An incomplete, but growing list of those IUPAC is aware of is on the IUPAC web site.
http://old.iupac.org/inchi/adopters.html#database

At the CPEP meeting I was asked if the Blue Book will have InChIs included.

One very important group to adopt InChI as the standard way to represent chemical structures is the EBI, as this puts InChI in the mainstream of the biological/medical world. Since Turin I have 6 official talks on InChI/InChIKey, many unofficial talks and meetings, as well as a video lecture at Google:
http://www.hellers.com/steve/pub-talks/

In addition talks with publishers (Nature, ACS, Elsevier, John Wiley, Thieme, and others) have been initiated and are continuing. Associated with these talks with publishers, at the CPEP meeting it was suggested that IUPAC ask the software drawing vendors who already support to add a feature to include the InChI/InChI Key in the output files they already create. In this way a user will be able to pass on the InChI/inChIKey to the publisher without any extra effort.

In October 2007 the InChI project joined the Microsoft BioIT Alliance of some 90 companies. I expect that Microsoft will adopt InChI as their chemical structure representation standard.
http://bioitalliance.org/
http://bioitalliance.org/blogs/iupac/archive/2007/10/03/222.aspx

A compressed InChI string has been developed, the InChIKey which is 25 characters long and makes web searching/lookup much easier.

Artus Labs, a small company in North Carolina, has indicated an interest in extending InChI and creating a 3D InChI. Plans are for myself and Tony Williams to discuss this with the Artus staff in August, as Tony, who is in North Carolina, knows these people.
http://www.artuslabs.com/

An IUPAC project proposal to "InChIfy" PAC has been submitted to IUPAC for funding. When asked about the details the folks in Prague, where the work is to be done, said it was really $38,000 to resolve the technical issues with going from structure on the PAC journal page to InChI. They did not plan to go from names to structures. Also they planned to test the computer system only on a few years of PAC, not all of PAC. I assume this will move forward this year. (All of PAC is now online and available. Anyone can get the back issues for free on the IUPAC web site, but access to the current year is via subscription only. *And* subscribers must go through a subscription agency – not the IUPAC web site.)

A meeting was held in Berlin in May to discuss expanding InChI to cover chemical reactions and develop an IUPAC XML standard – ReactML. (Minutes of that meeting, see Appendix C below.) The Berlin meeting had representatives of all but one major (who was represented by one of the attendees) and minor players who create/have or use (via software) reaction databases. One striking point of the meeting was that everyone said very clearly that using InChI was to be the starting point for the project as InChI is now considered *the* standard in the world for chemical structure representation.

Lastly, as Alan McNaught has pointed out, there is the serious and imminent question of how InChI development and maintenance should be funded in future – it is clear that there is a need for ongoing support for the type of service currently provided by NIST staff and Igor Pletnev in Moscow. The current existing IUPAC Project System does not seem well-suited to this kind of arrangement. Furthermore my term on Division 8 will expire in 2009 and there needs to be some working party or sub-committee established by Division 8 to oversee InChI, InChIKey, and ReactML activities. At the recent CPEP meeting, this general issue came up with respect to the need for an ongoing effort (maintenance) of the web site. It was agreed that the IUPAC

project mechanism was not appropriate for the ongoing web site work and plans are underway to request a budget for this be placed directly into the budget for the Secretariat. I propose that the same thing be done for the ongoing (bug fixing and maintenance) of InChI and related inChI activities. In conversations with Alan we propose to set up a separate InChI subcommittee. Suggested members would be Alan, myself, Tony Williams, Andrey, and perhaps an NCI or NIH person. As for Igor Pletnev, he is now getting $10,000 for the year from IUPAC. NIST is also proving funding, but that is not all for InChI.

I would also suggest the propsed subcommittee be the group to apply for project funds for InChI extensions, like ReactML, polymers, Markush, 3D, etc.

Appendix C

Minutes of meeting on IUPAC Computer Readable Chemical Reaction Database Standards held May 8–9, 2008 in Berlin, Germany, hosted by FIZ Chemie
July 30, 2008 – Stephen Heller

The goal of this meeting was to develop the requirements for a proposal to be submitted to IUPAC to fund an Open Source, public domain ReactionML (an arbitrary/initial name given to the current activity) standard to complement the IUPAC InChI chemical structure representation. That is, develop an InChI equivalent for reactions. The requirements would include what the community needs (that is, the content/data fields), technical and organisational issues and financial aspects. It is assumed that the current CML, developed by Rust and Rzepa, would be involved in the proposed project when it came to the form of the project. This meeting dealt with just the content part of the overall project.

Of those invited, 11 were able to attend. Those not attending had been sent a copy of the minutes for their comments and feedback. As of late July only 2-3 comments were received.

Attendance was as follows:

Guenter Grethe, Chair (ggrethe@comcast.net)
Stephen Heller, Secretary (steve@hellers.com)

Colin Batchelor, RSC (BatchelorC@rsc.org)
Bernd Berger, Wiley (bberger@wiley-vch.de)
Nick Chappell, Symyx (nick.chappell@symyx.com)
Kirill Degtyarenko, EBI (kirill@ebi.ac.uk)
Hans Kraut, InfoChem (Hans.Kraut@infochem.de)
Sandy Lawson, Elsevier (A.Lawson@elsevier.com)
Henry Matuszczyk, InfoChem (HM@infochem.de)
Axel Parlow, FIZ (parlow@fiz-chemie.de)
Martin Schmidt, FIZ (Schmidt@fiz-chemie.de)

Unable to attend/interested in project:

Jonathan Goodman, Cambridge (J.M.Goodman@ch.cam.ac.uk)
Guido Hermann, Thieme (Guido.Herrmann@thieme.de)
Joe Townsend, Cambridge (jat45@cam.ac.uk)
Bill Town, Kilmorie (bill.town@kilmorie.com)
Les Jordan, Microsoft (ljordan@microsoft.com)
Rudy Potenzone, Microsoft (rudolphp@microsoft.com)
Josep Prous, Thomson Reuters (josep.prous@thomsonreuters.com)
Martin Rothlisberger,Wiley (mrothlis@wiley.co.uk)
Shelly Rahman, Thomson Reuters (shelly.rahman@thomsonreuters.com)
Roger Schenk, CAS (rschenck@cas.org)
Steve Bachrach, Trinity (steven.bachrach@trinity.edu)
Chris Steinbeck (steinbeck@ebi.ac.uk)
Peter Murray-Rust (pm286@cam.ac.uk)
Henry Rzepa (h.rzepa@imperial.ac.uk)

Meeting agenda
Opening remarks by Rene Deplanque, Head FIZ Chemie
Introductions and interest in topic by attendees
Reasons for the project
Storing/registration vs. manipulation of information
Purpose of the meeting
Defining scope
Reaction types (organic, inorganic, kinetic, etc.)
Prioritisation
Format & definitions
Single and multi-step reactions
Metadata
Layered information
Applicable languages
Estimation of time and costs
Manpower requirement
Time frame for project
Agreement on plan of action and conclusion of meeting

After the introductions a number of the members of this task force working party discussed the many aspects and complications of chemical reactions. Over the course of the next few hours a clear consensus began to evolve that the IUPAC ReactML should be a standard, not a search system. It should only be a way to store and archive reactions. Within a very short period of time it was agreed that the RoadMap for developing the IUPAC ReactML should begin with two initial stages for the overall scope of the

project. It was also made clear to all in attendance that none of these proposed IUPAC activities should or will overlap with existing commercial and non-profit activities in these areas.

Conclusions
1. In the first stage there would be only the basic items and represented just as structural features (InChIs). The data items would include:

- reactant (i.e., left side of equation – all individual structures and combinations of all reactants)
- product (i.e., right side of equation – all individual structures and combinations of all products)

Above two should include, when available, mapping information and coordinates.

- reagent (structural info)
- catalyst (structural info)
- solvent (structural info)

Use a controlled vocabulary for the above three items.

- comment field - ??

It was felt that 9 months would be sufficient time to carry out this initial stage. Colin Batchelor, RSC, has been able to obtain RSC support for this first stage, with the actual work to be done in Jonathan Goodman's group at Cambridge. Work is expected to begin in the summer of 2008. The InfoChem participants offered the RSC test files to check the results developed. The working party members will test the algorithm. The group would plan a short write up for Chemistry International at the end of the test period. It was commended that the C language be used to be compatible with the InChI activities.

As part of the work software will be written to:
Convert RXN files to IUPAC ReactionML (RML)
Convert RD files to RML
Convert SD file to RML

2. Second Stage/Second Phase: After the first stage/phase has been tested and accepted work would begin on the second stage/phase, which will require resources not yet available. In order to do this a project proposal would be prepared and submitted to IUPAC for funding.

The additional data items for Phase 2 would include

Reaction worked – Y or N
Yield
Temp
Time
Concentration
Comment field
Reaction Type/Classification

Create an "anchor" atom
Atom mapping
Coordinates
Multi-step reactions
Factual data
Reaction tree

Estimated as a 2-year project.

Appendix D

Nomenclature for rotaxanes and pseudorotaxanes (Project 2002-007-1-800)
Report to IUPAC Division VIII Committee, August 2008 [AY; adapted by TD for the present minutes].

After long discussions and several rounds of review due to significant terminological problems it was decided to split the initial document into two parts: *Nomenclature for Rotaxanes and Pseudorotaxanes* and *Nomenclature for Stereoisomeric Rotaxanes and Pseudorotaxanes.*

The first part that discusses general principles of rotaxane nomenclature and "positional" isomerism of rotaxanes is accepted for publication in PAC and most probably will appear this year. [TD: has now appeared, cf. minute 8.3 above].

The splitting of the rotaxane recommendations in two parts has several advantages:

- The first general part is intended for a wider audience of rotaxane chemists and is free from specific stereochemical considerations that may be too complex for chemists not involved in this area.
- Earlier publication of general part of rotaxane nomenclature principles facilitates work with the dependent project on nomenclature of rotaxane polymers [TD: see minute 8.9.3 above].
- Separate consideration of stereoisomerism of rotaxanes allows more detailed consideration aiming at stereochemistry specialists.
- The task group will have more time to consult and decide about terminology of this area that needs involvement of other nomenclature experts.

The second part will be devoted to terminology of rotaxane isomerism and stereoisomerism with recommendations for specification of rotaxane stereoisomers.

Most fundamental terminological problems that must be solved in the second part are:

- Classification of "positional" and "orientation" isomers of rotaxanes. The current definitions do not distinguish one type from another.
- Isomeric rotaxanes have obvious relation to chemical topology that totally lack any terminology accepted by IUPAC. Topology-related terms may help in classification of rotaxane isomers.
- How to call rotaxane components lacking some principal symmetry element(s). There are several possibilities but currently all of them are absent or contradict with official IUPAC terminology.

More background is given in Appendix E below.

Appendix E

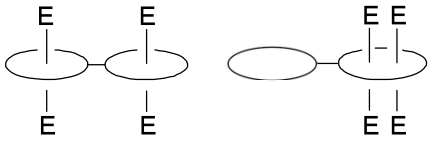
Project No. 2002-007-1-800
Nomenclature for rotaxanes and pseudorotaxanes, part 2
Terminological problems with rotaxane nomenclature – issues for discussion at task group meeting in Büdingen, Germany, July 30, 2008. [AY; edited lightly by TD for these minutes.]

Introduction
While preparing the recommendations for rotaxane and pseudorotaxane nomenclature, we met several terminological problems mainly connected with consideration of stereochemical properties of rotaxanes and their components. It was impossible to find a simple solution that did not contradict current IUPAC terminology and we decided to split the document into two parts:
General part – *Nomenclature for rotaxanes and pseudorotaxanes*
More special part – *Nomenclature for stereoisomeric rotaxanes and pseudorotaxanes*

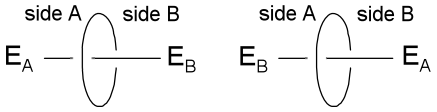
The first part was accepted for publication in PAC in April 2008 and probably will appear this year. [TD: It has now appeared, cf. minute 8.3 above]. The progress with the second part will depend on the terminological solutions to the problems found.

Consideration of terminology is the main subject of this task group meeting. Since consideration of rotaxane isomerism and stereoisomerism concerns general IUPAC terminology, several experts in general IUPAC terminology and terminology of stereochemistry are invited: Prof. Bernardo Herold, Dr. Ture Damhus, Dr. Karl-Heinz Hellwich. Another invited person is Prof. Jiři Vohlídal, chairman on the rotaxane polymers project.

Problem # 1
Let's look at the rotaxane isomers



and



"Type 1 Isomerism" "Type 2 Isomerism"

But according to IUPAC Gold Book:

> **Stereoismerism:** isomerism due to differences in the spatial arrangement of atoms without any differences in connectivity or bond multiplicity between the isomers.

It means that all considered isomers fall into category of stereoisomers and even our intended splitting of recommendation into "non-stereo" and "stereo" parts contradicts with current IUPAC terminology.

Our intuitive decision to treat isomers of Type 1 as non-stereo isomerism and of Type 2 as stereoisomerism reflects real chemical perception of stereochemistry that unfortunately is not reflected in IUPAC terminology.

The reason here is that classical IUPAC terminology does not take into account topological differences between molecules and does not have any topology related terms. But rotaxanes, catenanes and knots are common chemical objects that need consideration of molecular topology.

What options do we have? Several:
1. Still neglect need in topology consideration and classify these isomers as "positional stereoisomers" and "orientation stereoisomers".
2. Introduce new definitions of
   - **"topological isomers"** as "isomers having the same constitution but differing in their topology ignoring spatial arrangement of atoms"

   To separate topological isomers from stereoisomers we will need small modification of stereoisomerism definition: **isomerism due to differences in the spatial arrangement of atoms without any differences in connectivity, bond multiplicity and topology between the isomers**

   - **"topological stereoisomers"** as "isomers having the same constitution and topology but differing in spatial arrangement of atoms"

An introduction of topological isomerism already solves our problem but additional introduction of "topological isomerism" allows to distinguish classical stereoisomers and stereoisomers existing due to different topology of molecule.

So the solution of problem #1 needs a decision about introduction of topology terms in IUPAC terminology.

Problem #2
How to describe molecules that lack certain principal elements of symmetry?
This problem was the main reason for disagreement about the "stereochemical part" of the rotaxane recommendations.
For stereoisomers to exist for a rotaxane, its components need to lack rotational C_2 symmetry axes perpendicular to the linear section of the threading component or belonging to the nominal plane of the macrocyclic component.

Two main versions were used in the preliminary document:

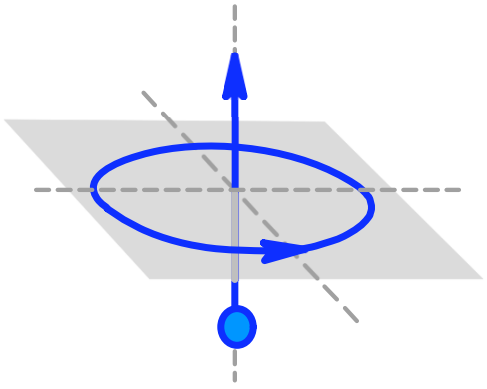
- Consideration of this symmetry property as a type of **asymmetry** that refers to absent symmetry element. This way was rejected as formally contradicting with IUPAC definition of asymmetry.
- Consideration of such components as **unsymmetrical**, i.e. not as asymmetrical, but as lacking just some symmetry property. This way was also rejected due to absence of such term in IUPAC terminology.

What options do we have here? Again several:

1. To introduce "unsymmetrical" term. But this term has some drawbacks that will be described in the presentation of Prof. Bernardo Herold.
2. To introduce new terms "unidissymmetrical" and "bisdissymetrical". These terms were proposed by Prof. Bernardo Herold during participation in the review of rotaxanes recommendations and he will explain these terms and other possibilities in his presentation during our task group meeting.
3. We also can consider another option that formally does not introduce any terms but refers to "low dimensional asymmetry and chirality". This proposal will be illustrated in more detail in a special presentation by Andrey Yerin. Here we give just short basic description of this idea.

This way may be based on the consideration of stereoisomeric rotaxanes and their component according to their dimensionality and symmetry properties in 1D and 2D spaces.

For example let's look at familiar figure with "cyclochirality":



It is clear that this schematic representation of one enantiomer of a rotaxane has a composite stereogenic unit formed by two components:

- linear (1D) component that defines direction along line
- 2D component that defines circular direction.

Fixed perpendicular orientation of 1D and 2D components creates composite 3D stereogenic unit. We may take it as a starting point for consideration of 1D and 2D stereogenic units and 1D and 2D asymmetry. Is consideration of low dimensional asymmetry so strange and uncommon? Hardly! For example we may find in V. Prelog and G. Helmchen, *Basic Principles of CIP-System and Proposals for a Revision*, 1982:

"It is possible to apply the concepts of chirality and chirality sense to spaces whose dimension is either less or more than three. In fact, discussion of two-dimensional chirality can lead to better understanding of three-dimensional stereoisomerism."

So low dimensional chirality and asymmetry are logical and even useful part of stereochemistry.
Following this way we may call the components of rotaxanes that may form rotaxane stereoisomers as: 1D asymmetrical and 2D asymmetrical or possessing 1D and 2D stereogenic units, thus referring to an absence of symmetry elements in relation to a specific axis or plane.

The progress of the second part of the rotaxane recommendations significantly depends on our solutions of the two main terminological problems and we may hope that this task group meeting may allow us to move further in rotaxane nomenclature and terminology. The decisions made here will help also for such close areas as catenanes and knots.

Appendix F

Draft minutes of the annual meeting of the Nomenclature Committee of the IUBMB (NC-IUBMB) and the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN), Copenhagen, Denmark, May 16-17, 2008

Attendees:
NC-IUBMB and JCBN
Keith Tipton (Dublin, Ireland)
Hans Vliegenthart (Utrecht, The Netherlands)

NC-IUBMB

Dietmar Schomburg, Chairman (Braunschweig, Germany)

JCBN

Sinéad Boyce, Secretary (Dublin, Ireland)
Gerard Moss (London, UK)

Database Representatives
Wim Vranken (EBI, UK) – PDB representative
Rolf Apweiler (EBI, UK) – UniProt representative

Others

Derek Horton (Washington, DC, USA)	
Kristian Axelsen (Copenhagen, Denmark)	Observer
Sabine Kuhn (CAS, Columbus, OH, USA)	Observer
Ture Damhus (Copenhagen, Denmark)	Observer (Novozymes and Secretary of IUPAC Division VIII)
Lars Henrik Østergaard (Copenhagen, Denmark)	Observer (Novozymes)
Karl-Heinz Hellwich (Offenbach, Germany)	Observer (IUPAC Division VIII)

1. Welcome and Apologies

Before the meeting started, Damhus gave the committees a brief introductory talk about Novozymes and outlined the general arrangements for the day. Novozymes has 4500 employees and is the largest industrial enzyme supplier in the world. It originated in Novo Nordisk but became a separate company in 2000. A guided tour of two of the Novozymes facilities, of which there are many, was arranged for the period after lunch. These were the plant in which pilot-scale production of enzymes is carried out to determine optimum conditions prior to full-scale production and the bakery-enzyme laboratories.

Schomburg gave a presentation to the committees and to some interested parties from Novozymes on the work of the committees, the classification process etc. This was followed by a questions and answers session.

Schomburg thanked Damhus and Axelsen for organizing the meeting and for making such excellent arrangements. Apologies had been received from Cammack, Cantor, Chester, Degtyarenko, Dixon, Kanehisa, Kazic, McNaught and from Prof. Willy Stalmans, of the IUBMB Executive Committee, who had been invited to attend the meeting.

2. Approval of the Agenda

Schomburg had two questions regarding the agenda. The first concerned a suitable time for the carbohydrate experts (Vliegenthart, Moss, Horton and Hellwich) to hold a separate meeting to discuss differences of opinion regarding the necessity for a revised carbohydrate document and its possible content. As this was arranged for the evening of May 16, Item 7.2 was to be deferred until May 17 for discussion. As Wim Vranken, Berman's replacement representative, was unable to attend on May 17, items that concerned PDB were to be discussed on May 16 (Items affected were 7.5, 8.9, 8.14 and 8.15). He also wanted to raise a point about peptide hormones (added to agenda as Item 8.17). Another item to be included on the agenda was the question of stop codons (this was added to the agenda as Item 7.12).

3. Minutes of the Chevy Chase Meeting, May 2007

Minutes of the Chevy-Chase meeting were approved.

4. Matters Arising

There were no matters arising. Vliegenthart reported that Bengt Lindberg, a former member of the committee, had died and Tipton informed those present of Hal Dixon's ill health. It was decided to pass on the good wishes of those at the meeting to Hal, so a card was circulated and signed by all.

5. Reports

5.1 Chairman's Report (Schomburg)

Schomburg gave a brief report on some of the activities of the committees. He was allowed to sign the memorandum of understanding with CAS on behalf of the IUBMB and the initial exchange of data has taken place. Moss and Boyce have implemented the changes to CAS numbers as a result of this and the Enzyme-List data have been sent to CAS as an XML file.

Computer programs have been developed by Schomburg's group to compare the Dublin and London versions of the Enzyme List and to compare the Dublin and IntEnz versions of the Enzyme List.

Transcription factors – Schomburg reported that he had written to the TRANSFAC group asking them to produce a document on the classification of transcription factors. Despite repeated reminders, this has not yet been done.

Cammack had sent Boyce an outline version of the newsletter and asked for notification of any modifications to be made, if required. Each person at the meeting received a copy of the newsletter to review and it was discussed under item 7.10. Suggestions for further inclusions should be submitted within three weeks (by June 15). It was reported that the newsletter will, in future, take the form of a rolling newsletter, with single items being added to a web-based version as and when they are drafted and approved.

UniProt protein-naming guidelines. This document was discussed at the 2007 meeting and should be re-read by the committees. Any problems, suggestions etc. should be e-mailed to Schomburg by June 19. (**Action:** Boyce to send out latest version of the UniProt document to those at the meeting).

5.2 Treasurer's report (Cammack)

Cammack was unable to attend the meeting and did not provide a Treasurer's report. He did, however, send an e-mail to Boyce and Schomburg in March 2008, which stated that the amount remaining in the IUBMB account for the current triennium (2006-2008) was $3217 USD, with a further $2000 being promised by Jan Joep de Pont, IUBMB treasurer, for this period.

6. Enzyme Nomenclature and Classification

6.1 Progress report on the classification of enzymes and dissemination of enzyme data (Boyce, Tipton)

(a) Energases. Tipton reported that these enzyme entries will be ready for public review in the near future.

(b) Amine oxidases. These are on the agenda as they represent an anomaly, having been classified on the basis of containing either copper or flavin, which is not the normal basis for classification. Tipton reported that he has proposals for reclassifying these enzymes that will go through the review process in the near future, along with some other amine oxidases, such as bacterial methylamine oxidase.

(c) Carbohydrate enzymes

Enzyme entries have been modified so that an arrow rather than a comma is used to indicate the atoms of disaccharides that form the linkage (e.g. '1,3' has been changed to '1->3'). This change has been implemented in the reactions and systematic names in accordance with the Carbohydrate-document recommendations although some still need to be done (**Action:** Boyce to check the Enzyme-List for any cases that should have been changed but were overlooked). Moss said that the specification is missing in some cases and a search of the literature would be required to ascertain the correct designations. Horton will check the Enzyme List in June 2008 to ensure that all necessary changes have been implemented.

7. Items for Discussion

7.1 Presentation of a pilot project on a glossary of enzyme-chemistry terminology (Ture Damhus and his colleagues Prof. Bodil Nistrup Madsen, Annemette Wenzel, Peder Olesen Larsen) followed by discussion of a prospective IUPAC/IUBMB project on this work.

This project began as an initiative from the nomenclature committee of the Danish Chemical Society, and involves Ture Damhus, Ph.D., Peder Olesen Larsen (Dr. Phil. et Dr. Scient.), and from the DANTERM terminology centre at the Copenhagen Business School, Prof. Bodil Nistrup Madsen, a computer linguist, and Annemette Wenzel, a computer linguist.

The aim of the project is to create a codified Danish chemical terminology, i.e. a concise definition of terms, for chemistry and biochemistry concepts. In order to do this, they are creating an ontology/concept-based English terminology, starting with the narrower field of enzyme chemistry. They have found that terminology is not always consistent and well defined, and gave the Gold Book as an example, pointing out that many terms one would expect to find there are missing. Examples of such terms are: amino-acid derivative, molecular structure, glucosylation, glycation, inactivation, proenzyme, zymogen, genetic engineering and enzyme complex.

Examples of concept diagrams in the i-Term terminology and knowledge management system were presented and a demonstration can be seen at http://www.i-Term.dk. Inheritance can be introduced into the system and a polyhierarchy is also

used. Custom fields for both concepts and terms can be added, with each term having a general definition. Examples of the concepts included in the i-Term terminology include alpha-helix, beta-pleated sheet, molecular structure, primary structure, secondary structure etc. A feature specification is that one must have an attribute-value pair, i.e. cannot have the same attribute with different values. It was pointed out that the terms primary, secondary and tertiary structure were often poorly defined and contradictory.

The data sources used to date are the IUPAC Gold Book, The Oxford Dictionary of Biochemistry and Molecular Biology (2nd ed.), Wikipedia and some Danish sources. Damhus would like to know of other sources that could be used to obtain terminology. Damhus said that we, as the nomenclature committee, should feel a responsibility in the area of biochemical terminology and he suggested that we need to do more work.

A discussion of the value of the project and the way in which the JCBN could get involved ensued. Moss said that the JCBN could be proactive and look at terms in the Gold Book to see if they are appropriate/adequate. Definitions that may need revision could be identified and definitions could be provided for those terms that were found to be absent. Damhus said that they have only used approximately 100 terms to date, whereas the Gold Book has about 6000 terms. Vliegenthart said that many terms other than alpha-helix and beta-sheet should be included in terms of secondary structure. Damhus replied saying that what they presented was just a preliminary draft and that they intend to include other terms. Tipton said that we should see if this work could become an IUPAC or IUBMB project. Moss made the point that ICSU funds international projects that are interunion and said that it may be worth investigation by Damhus. Moss said that it should start off as a limited project by selecting those terms that are most frequently required, but with room for expansion. Schomburg asked if there was a time-scale for the project but no timescale was given (**Action:** Damhus to investigate the possibility of funding this project through ICSU and to advise JCBN of what he would like committees to do; anyone with suggestions for data sources that could be used in iTerm project to contact Damhus - TDa@novozymes.com).

7.2 Update on the revision of the carbohydrate document (Horton, Vliegenthart)

The Carbohydrate group held a one-hour meeting and devised a plan of action to draft a revised carbohydrate document that is specifically aimed at biochemists. The first objective is to get the project registered with IUPAC. The plan is to expand specific sections of the old Carbohydrate document, starting with the oligosaccharides and to add new material on the basics of carbohydrate structure. Horton will write the preamble. The section on common trivial names (names ending in -ose or -an) and the corresponding systematic names can also be expanded. The trivial names for compounds from non-standard monosaccharide parents, e.g. basilose, will also be revised and expanded. Some problems with the nucleotide sugars and with the way that phosphates are designated will also be addressed. It is also planned to expand the section on glycoproteins to include such terms as glycoclusters, glyconanoparticles and glycodendromers. The CFG system may be incorporated as an example of a pictographic form for depicting carbohydrate chains.

If the project is approved by IUPAC, the plan would be for the subgroup to meet in late autumn of 2008, so that they can iron out any problems. Horton plans to ask Alan McNaught to participate in the project (**Action:** Horton to draft application to IUPAC for project approval, to write the preamble and to ask Alan McNaught if he will be involved).

Regarding the glossary, Damhus urged that the project members make a connection between the main text and the glossary. He said that, in IUPAC, they have made the decision to use only three qualifiers for names: preferred names, acceptable names and not-acceptable names. He said that the document Graphical Representation Standards for Chemical Structures adheres to this system.

The topic of glucitol was raised. Tipton said that, among biochemists and medics, glucitol is always referred to as sorbitol so it would be difficult to say that sorbitol is not an acceptable name. Tipton said that he would prefer it to be an IUPAC recommended name. Hellwich said that a 1996 document has already said that sorbitol should not be used. Damhus said that we should say that sorbitol is acceptable and that perhaps IUPAC need to revise the 1996 decision to say that it is acceptable.

Any correspondence on revision of the carbohydrate document is to be sent to the JCBN mailing list (jcbn@qmul.ac.uk).

(a) Symbols for monosaccharides (Tipton)

Tipton showed a slide of N-glycan carbohydrate structures comprising the symbolism used by CFG (Consortium for Functional Glycomics) and by UOXF (Oxford Glycomics Institute), along with a text version. He asked the carbohydrate experts to consider which of these systems we should use. Vliegenthart said that the CFG method is better suited to mass spectrometry as the colour of the symbols gives an indication of molecular weight. Horton said that neither of the systems expands to cover all of the carbohydrates for which symbols might be required. While the CFG system was developed for glycoproteins, Vliegenthart said that it could also be used for glycolipids. Damhus said that differentiating on the basis of colour has a disadvantage for colour-blind people and he therefore objects to the practice. Tipton pointed out that there were both colour and grey-scale versions of the CFG symbols. Vliegenthart said that he liked the wording that Cammack used in his draft newsletter (under the item 'Iconic symbolism for carbohydrate nomenclature').

7.3 Update on the phosphorus document (Moss)
The document was slightly updated since the last meeting. Moss reported that, as the new Blue Book had not been published as expected, the references would need to be changed. Moss will finish off the document and submit it to IUPAC. Moss mentioned that there is a new discussion board on the new IUPAC website so he is not sure who will receive the document (**Action:** Moss to finalize phosphorus document and submit it to IUPAC).

7.4 Update on the cooperative effort between CAS and NC-IUBMB (Schomburg, Kuhn)
A document of understanding has been signed. Kuhn reported that she had sent the CAS numbers to Boyce, Axelsen and to Rafael Alcántara of the EBI. She had carried out a mapping of CAS numbers to EC numbers and provided a document (attached) indicating that there is not a 1:1 correlation in all cases, e.g. ATPases (where CAS has collected ATPases at two RNs and IUBMB has split them into many EC numbers) or protein kinases (where CAS has split kinases, whereas IUBMB has collected them together). Disparities in approaches between CAS and IUBMB for these enzymes have to be resolved at CAS. Moss said that it would be useful to include the CAS index-heading name as a synonym in the Enzyme List. Tipton agreed that it would be useful to have these names and Kuhn said that she could get these but that there needs to be an exchange of data. (**Action:** Kuhn to send index-heading names used in CAS to Boyce and Moss for inclusion as synonyms in the Enzyme List)

Kuhn said that she would like to get Enzyme-List updates from the Dublin group in a pre-defined timeframe. Tipton said that that would be easy to do (**Action:** Kuhn and Boyce to discuss CAS's requirements and to agree a timeframe).

Tipton asked if CAS acknowledge that enzyme data can be from the IUBMB. Kuhn said that this hasn't been addressed. Tipton said that it would be useful to have some mention and Moss suggested Appendix IV to the Index Guide as a suitable place for such an acknowledgement.

7.5 Update on the small-molecules project (Cammack)
Schomburg said that the small-molecules project should be conducted in close collaboration with ChEBI and that Cammack should also check if the participants listed as project members still wish to be involved. Moss said that the small-molecules document should cover small molecules that are encountered quite regularly but where there is no document giving the numbering of atoms and details of how to name modified versions of the compound. Tipton said that numbering of atoms in small-molecule structures would be extremely helpful. Riboflavin, thymine diphosphate and coenzyme A were given as examples of the compounds that Moss had in mind for inclusion. Hellwich said that he would like to be added to the list of those consulted about this document. Vranken said that John Westbrook of PDB should also be included as a project member but he believed that Cammack had already written to Helen Berman about this. (**Action:** Boyce to send additional names to be included as project members to Cammack and to ask him to double-check with those already on his list to ensure that they are still available to contribute to the project). Schomburg reminded the committee that what is to go into this document was mentioned in the 2006 minutes.

Hellwich suggested that we should update the document on nucleosides and nucleotides. Moss said that we had talked about going through the White Book and determining which documents should be revised. Schomburg wants a volunteer to push this proposal. Moss would like to be involved in the small-molecules document but would not have a lot of time to do the writing.

7.6 Membership of Committees
Schomburg wants people who provide expert assistance to be named on the website as consultants and not necessarily to retain their membership/associate membership. Charles Cantor has been removed from the list of members. Schomburg said that project members do not have to have involvement with either a Division or the committees, i.e. there should be someone from the JCBN on a project committee but others involved need not be members of the JCBN.

7.7 Progress report on the work of the thermodynamics panel chaired by Bob Alberty (membership: Athel Cornish-Bowden, Robert Goldberg, Gordon Hammes, Keith Tipton and Hans Westerhoff).

Tipton showed a slide of the 'Recommendations for Nomenclature and Databases for Biochemical Thermodynamics' document, which had been distributed to those on the JCBN mailing list (sent as Item_7.5.pdf in April 2008). The completed document was sent to IUPAC, who returned it saying that it could not be called nomenclature as it refers to terminology. The IUPAC referee, Prof. Jack Lorimer, also objected to usage of several terms that had been used within the document, such as M and molarity, saying that mol dm^{-3} or mol L^{-1} should be used instead. Alberty had said that they might have to produce one document for biochemists and another one for IUPAC but this was not recommended by Lorimer. Tipton and Bob Goldberg are trying to produce a version of the document that might be acceptable to all concerned. Damhus, who worked for four years under Lorimer, said that Lorimer is quite agreeable to having a discussion about differences of opinion. Moss offered to liaise with Lorimer over the differences of approach.

Schomburg suggested that those terms used in the document that do not adhere to strict IUPAC nomenclature should be accompanied by a footnote giving the IUPAC term but pointing out that the document is primarily for biochemists. He said that

the name of the document is the same as that of the previous document that it is replacing so it would be better to retain the 'nomenclature' version of the title although he has no strong feelings on the topic. (**Action:** Tipton to provide Moss with a copy of the slides he had prepared on the major points of difference and copies of the correspondence on this matter so that he can contact Lorimer about these issues).

7.8 Liaison with IUPAC (Tipton)

Tipton mentioned an error report that Athel Cornish-Bowden had submitted to the editor of the Green Book, who said that it was too late to correct the error. Since this error concerned enzyme kinetics, Cornish-Bowden believed that the compilers should have consulted the committee before it was included. Damhus said that there was a five-month public-review period so that everyone should have had ample time to notify the editors of any errors.

7.9 Update on the work of the STRENDA Commission (Schomburg, Tipton)

STRENDA is making progress in several areas and is now associated with the MIBBI (Minimum Information for Biological and Biomedical Investigations) group (http://mibbi.sourceforge.net/). The paper describing the STRENDA initiative needs to be revised before being accepted by Nature Biotechnology (**Action:** Schomburg to send Tipton the final version for him to revise). Tipton said that the main aim of STRENDA was to ensure that authors provide full details of the methods and conditions that they used when publishing enzyme-related data. To this end checklists had been prepared for the guidance of editors and referees (available at http://www.strenda.org/). This has received favourable responses from several journal editors. The next step is to encourage people carrying out experiments to standardize experimental conditions for a particular organism if they want their data to be of value in systems biology. However, the design of organism-specific checklists requires advice from experts in the different areas. A related activity is to design forms for data submission that could be incorporated directly into databases. Draft forms were developed but they were rather elaborate. Tom Leyh, a member of the commission, is currently trying to design a simpler form. There will be another conference in September. Apweiler is leaving the STRENDA commission, to be replaced by Christoph Steinbeck (EBI).

7.10 Items for, and publication, of a newsletter (Schomburg)

A copy of the newsletter, prepared by Cammack, was distributed to those at the meeting. Schomburg went through the newsletter item by item at the meeting and items to remain were as follows: (a) the use of gene symbols for gene products, (b) accepted name, (c) partial EC numbers, (d) pyrrolysine, (e) lipid classification, (f) metabolic charts, (g) IUPAC publications of interest to Biochemistry and Molecular Biology. Moss asked that the colour be removed from the diagram of pyrrolysine. In future, individual items will be added to the newsletter as and when they arise. It was agreed that there would be a committee-review period before newsletter items are made public (**Action:** Schomburg to revise item (a), Boyce to revise item (b) and anyone with an item to include should send it to Boyce; Boyce to coordinate this activity and Horton to be involved).

In answer to a question regarding other items that should be included in the newsletter, Hellwich mentioned the item on doubly substituted peptides that he had submitted in 2006. (**Action:** Boyce to resend item on doubly substituted peptides to McNaught and Moss for review). McNaught had drafted an item on locants in 2006, for inclusion in the newsletter but the decision to change the way that locants are written was rescinded in 2007 (**Action:** Boyce to include global-change information on website saying that the previous decision was reversed). There are new recommendations from Division VIII on drawing structures (133-page document) and another document on stereochemistry. Moss said that we should have a newsletter item notifying biochemists of these publications (**Action:** Moss to write newsletter item).

7.11 Operation of the JCBN – how to improve output and communication

(a) Integration of additional scientists in the work of the JCBN

Discussed as part of Item 7.6.

7.12 Stop codon

Schomburg said that a way of describing modifications of protein sequences that either insert a stop codon or have insertions or deletions should be found. Apweiler said that, in their databases, they state where the change occurs. A more complex question is to define the original reference point (one gene can give rise to many translated transcripts), which can also have post-translational modifications. There would have to be descriptors for a whole cascade of changes made to the transcript at an amino-acid level. The latter problem cannot be solved before coming up with a proper nomenclature for the whole process. Apweiler said that one could use protein identifiers, e.g. UniProt accession numbers, and indicate changes from the reference object. We have been asked to provide a three-letter and a one-letter code for a stop codon. Schomburg has seen a protein accession number followed by a Delta and the numbers of the amino acids that have been deleted e.g. D110-150. A stop codon indicates the end of an amino-acid sequence so this might be covered by changing the number of amino acids. Moss said that part of the amino-acid document deals with the modification of peptides. Østergaard said that, in Novozymes, they indicate additions and deletions as follows:

W361T – substitution

W361* – for deletion of a single amino acid

361aT – for addition of another amino acid after position 361

A request had been received from Professor Wen-Chang Chang (University of Taiwan) for a recommendation regarding usage of the term codon. The term originally referred to mRNA but is now being used to refer to DNA as well, which can lead to confusion. Normally, the codon is considered to be on mRNA and the anticodon on tRNA. These are sometimes referred to as the Watson strand and the Crick strand, respectively. Apweiler said that we should consult with people in the genomics field and see how they use the terms (**Action:** Apweiler will ask Alex Bateman about nucleic acids and to draft definitions for non-coding RNAs). Apweiler also suggested that Elspeth Bruford, who is the coordinator of the HUGO Genome Nomenclature Committee (HGNC) and is located at the EBI, be asked to look into insertions, deletions and mutations, and to make a recommendation for use at the protein level (**Action:** Apweiler to ask Elspeth Bruford for a suitable recommendation). She could also be asked to come up with a definition for "codons" on DNA and could then be asked to bring the recommendations to the annual meeting in 2009.

8. Update on Action Items from the Minutes of the 2006 Meeting

8.1 Schomburg to sign a letter of agreement with CAS (Minute 5.1: Action by Schomburg)

This has been done.

8.2 Schomburg to draft acknowledgement and to consult database curators having finalized wording with Boyce; Boyce to send Schomburg a list of databases that use the JCBN data extensively asking them to acknowledge our work as the source of some of their data (Minute 5.1: Action by Schomburg, Boyce)

This has not been done yet.

8.3 Boyce to undo all changes made to locants for amino acids in the Enzyme List (Minute 7.1: Action by Boyce)

This has been done.

8.4 Those with suggestions for items to be included in Jeff Leigh's "Principles of Chemical Nomenclature" to forward them to Moss (Minute 7.2: Action by all)

Moss received none. Damhus pointed out that this is a basic book for students and teachers so he was disappointed that the JCBN did not participate, although he said that we still have time to do so (however, Moss and Dixon are both members of the nomenclature committees). Dixon was to be the second reader of the chapter on biochemical nomenclature but this may need to be reviewed. The topics covered in Chapter 7 of Jeff Leigh's book (http://old.iupac.org/publications/books/principles/principles_of_nomenclature.pdf) are carbohydrate nomenclature, nomenclature and symbolism for amino acids and peptides, lipid nomenclature and steroid nomenclature (**Action:** anyone with suggestions for additional items to include in this chapter to contact Moss).

8.5 Anyone with a suggested alternative to the term 'alloprote' to contact McNaught; Moss or McNaught to send a CHMINF-L e-mail on the subject (Minute 7.4: Action by all; Moss or McNaught to sent e-mail)
This should be done but no information on its status was available {Note: In his document "other items, not decided" that accompanied the outline newsletter, Cammack had suggested ASPROT(s) [Alternate state(s) of protonation] as a possible term}.

8.6 Moss to circulate recommendations for naming antisense oligonucleotides to be included in the phosphorus document and the committees to send him comments on his recommendations by e-mail (Minute 7.5: Action by Moss)

This has been done.

8.7 Schomburg's programmer/students and Andrew McDonald to work on the production of software to compare the qmul and Enzyme Database datasets (Minute 7.6: Action by Schomburg, McDonald)

This has been done.

8.8 Schomburg to compile a list of projects that will be published on the website along with the members involved in each project (Minute 7.7: Action by Schomburg).

This has not been done because a list of projects has not yet been compiled.

8.9 Boyce to draft letter for distribution to PDB staff on what is needed to classify a new enzyme; Axelsen and Berman are to coordinate the data that they will send to Boyce; Kanehisa to send new enzymes plus associated references to Boyce for inclusion in the Enzyme List (Minute 7.4: Action by Boyce, Kanehisa, Axelsen and Berman)

Boyce has not yet drafted the letter for PDB because of a large influx of new enzymes, especially terpenoid enzymes drafted by Moss, and Tipton agreed to draft the letter in consultation with her.

8.10 Cammack to compile list of topics to include in each of the newsletters and to consult with members of the committees about the content of these newsletter items (Minute 7.11: Action by Cammack)

This has been done.

8.11 Kanehisa to send Boyce his list of PMID numbers to include in the Enzyme List (Minute 8.1: Action by Kanehisa)

This has been done.

8.12 Schomburg to invite Bernard Henrissat to the 2008 meeting as an observer (Minute 9.20: Action by Schomburg)

Schomburg will invite Bernard Henrissat to the meeting in 2009 but, unfortunately, will be unable to pay his expenses.

8.13 Schomburg to request online access to BAMBED again for members of the committee (Minute 9.25: Action by Schomburg)

Schomburg has done this but did not receive a response.

8.14 McNaught, Schomburg and someone from PDB to be included in the working group on small molecules. Cammack to submit an application to IUPAC for project approval when preliminary investigations have been completed and to distribute the output to the committees by 8 February 2008 (Minute 9.3: Action by Cammack)

Cammack is currently drafting the project proposal to submit to IUPAC for approval.

8.15 Axelsen, Berman and Kanehisa to consider drafting a document on general guidelines for naming proteins using the UniProt document that was distributed with the 2006 Minutes (Minute 11.3: Action by Axelsen, Berman and Kanehisa)

This has not been done. Boyce is to send the latest draft of the UniProt document (available at http://beta.uniprot.org/docs/nameprot) to those at the meeting. Schomburg will wait for 4 weeks for any objections/suggestions.

8.16 Schomburg to ask TRANSFAC group to draft a paper on transcription factors (Minute 11.4; Action by Schomburg)

This has been promised but has not yet been received.

8.17 Peptide hormones. Vranken reported that, at PDB, there is a cut-off at 24-residues (i.e. sequences must be longer than 24 residues to be included) so PDB no longer deals with many peptide hormones. BMRB (Biological Magnetic Resonance Bank; BioMagResBank; http://www.bmrb.wisc.edu/) should be contacted instead. (**Action:** Schomburg to contact BioMagResBank and determine if there is a suitable person there to liaise with). The peptide-hormone document from 1974 is still being consulted approximately 150 times a week so it really needs to be updated. Tipton pointed out that most gut hormones do something different in the brain so saying that they are hormones is only telling half the story. He asked if a list of the differing functions of these hormones is required.

9. Funding Situation and Possibilities (Cammack)
9.1 IUPAC
9.2 IUBMB
9.3 Other possibilities
In the absence of Cammack, this was not discussed

10. Any Other Business
(a) Lyases. Tipton reported that it is often quite difficult to decide if an enzyme should be classified as a hydrolase or as a lyase and mentioned a pre-published paper by Diogo Latino, Qing-You Zhang & João Aires de Sousa (Lisbon) that had also found some problems in this class. He also said that Kanehisa's E-zyme program had had serious problems trying to predict the EC class for lyases. Tipton said that all of the lyases, and particularly the hydro-lyases, need to be looked at to see if any should be moved to a different class and he said that he would like some help with this task. Volunteers were requested. Schomburg said that he would run the lyases through his program (**Action:** Schomburg to liaise with Boyce and Tipton on the results of this analysis).

(b) Tipton showed a statistics table on usage of the Nicholson minimaps website (http://www.iubmb-nicholson.org/) and passed on Don's good wishes. He also reported that Sigma-Aldrich paid an unspecified sum of money each year to the IUBMB for the use of the material, which is IUBMB copyright. Nicholson had indicated that Sigma-Aldrich wished to reduce the amount paid substantially and asked Schomburg to find out from the IUBMB what their attitude to this might be (Action: Schomburg to contact IUBMB about the Nicholson maps).

(c) Enzyme-Nomenclature Book. Schomburg reported that Willy Stalmans is now responsible for IUBMB publications. Schomburg had referred Stalmans to Cammack and there had been an exchange of e-mails. The conclusion was that something should be done but Schomburg has not heard anything since. Schomburg recommended that we do nothing about it, at least for the time being. The general feeling was that there wasn't a general requirement for such a publication. Tipton mentioned that a LaTex version of the entire book or of any selected fields can be printed or saved using the print facility on the ExplorEnz website (accessible from any results of a search; http://www.enzyme-database.org/index.php).

(d) Tipton suggested that the committee should consider updating many of the items in the "White Book" (Biochemical Nomenclature and Related Documents). This was last published (2nd Edition) in 1992 and many of the items needed revision and updating. Moss said that the "White Book" was no longer available but each of the documents from it together with some more recent material and newsletter items were available on the web (http://www.chem.qmul.ac.uk/iupac/bibliog/white.html).

(e) Schomburg would like to get the statistics on the number of enzymes being submitted for classification correct. He had estimated that approximately 12 new enzymes are received from the public each year (**Action:** Boyce to check this figure). He also wanted to know the number of submissions from KEGG, PDB and MetaCyc in the last three years (**Action:** Boyce to determine the number of enzymes in each of the former categories).

(f) Damhus asked if IUPAC names could be included in glossary entries.

11. Date and Place of Meeting in 2009

The next meeting will be held in Braunschweig on 1-2 May 2009.

12. Open Forum

There were no items for discussion, other than those reported elsewhere in these Minutes.

13. Presentations (time allowing)

13.1 New developments made within the IntEnz project: a reaction database called Rhea (Axelsen)

Axelsen gave a brief presentation on the current status of the reaction database Rhea. One of the aims of the project is to deconstruct reactions that are text strings into reactants and products and then to link the compounds involved in ChEBI and to KEGG reaction IDs. He said that identifiers for reactions are stable i.e. the same reaction will have the same ID even if the EC number is changed.

The following tasks have been completed:

- The curator tool is working
- IntEnz reactions have been parsed into Rhea, and links between IntEnz entries (EC numbers) and Rhea reactions have been preserved.
- All of the reactants have been mapped to ChEBI compounds.

Tasks that are in progress include:
Reactions are verified and balanced for chemical content and charges using their charge-balance checker.
They have made the decision to use uncharged compounds as much as possible, so, carboxylate, for example, will be changed to carboxylic acid in reactions.

Rhea-specific names are chosen in ChEBI when several names exist (e.g. CoA or CoA-SH or CoASH). These names can be changed in ChEBI by Rhea curators. Cross-references are added to KEGG and MetaCyc reactions, and PubMed references are added for new reactions.
CheEBI curators create and update ChEBI compounds as needed.

Some figures:
Total number of reactions in Rhea: 3891
Number of approved reactions: 2008
Total number of compounds in Rhea: 4185
Number of compounds that are linked to ChEBI: 3648

The next steps to be undertaken are to prepare the public-release version and a public interface. The reactions in IntEnz will be changed to those in Rhea (so will no longer match Enzyme-List data)

Axelsen said that he plans to report changes to IUBMB and to include information on:

- reaction errors
- errors in reaction stoichiometries
- inconsistencies in the names of compounds used in the Enzyme List

(**Action:** Boyce to let Axelsen know the format in which to send these data).