Minutes of the IUPAC Chemical Nomenclature and Structure Representation Division (VIII) Committee Meeting

Prague, Czech Republic, September 6-7, 2006

Members present: Mr Jonathan Brecher, Prof Richard Hartshorn, Dr Stephen Heller, Dr Karl-Heinz Hellwich, Prof Alan T. Hutton, Prof Richard G. Jones, Dr Jaroslav Kahovec, Prof G Jeffery Leigh**,** Dr Alan D McNaught (Past President), Dr Gerard Moss (President), Prof József Nyitrai, Dr Warren Powell (Secretary), Dr Jeffery Wilson, Dr Andrey Yerin

National Representative Present: Dr Martin Ragner (Sweden)

Observers: Dr William Town, in part (Project Leader, Graphical Representation Standards)

Members Absent (excused): Dr Ture Damhus, Prof Franco Cozzi

The sixth meeting of the Division Committee of the IUPAC Division of Chemical Nomenclature and Structure Representation hosted by the Ústav makromolekulární chemie, Akademie věd České Republiky was convened by President Moss at the Hotel U Hvězdy in Prague, Czech Republic at 9:00 on September 6, 2006.

1.0 President Moss welcomed the members to this meeting and offered a special welcome to Dr. Martin Ragnar (National Representative from Sweden). Each of the attendees introduced himself and provided some background information. Housekeeping details regarding breaks and lunch were announced. Tomorrow's meeting (Sept. 7) will convene at the Institute; transportation will be provided from Hotel U Hvězdy.

2.0 Dr Moss noted that apologies for absence had been received from Members Dr Ture Damhus (who had sustained a damaged knee), Prof Franco Cozzi; and Prof Dietmar Schomburg (JCBN); and the National Representatives Prof Farxana Ansari (Pakistan), Prof Ivan Dukov (Bulgaria), Prof S Krishnamurthy (India), Prof Len Lindoy (Australia), Prof Jan Reedijk (Netherlands), and Prof Rita de Rossi (Argentina).

3.0 The agenda as circulated was approved with the addition of the following topics:

(1) Consideration of the manuscript "Improving the Quality of Published Chemical Names with Nomenclature Software" by Garnot Eller.

(2) A call for tenders on scientific and technical assistance for Scientific Customs from Herve Schepers.

(3) Problems with inorganic polymers

4.0 Minutes of the Beijing meeting.

The following are corrections (other than typographical errors) and changes to the minutes of the Division Committee meeting in Beijing that were posted on the Division VIII Webboard.

(1) Minute 2.0 line 4. Read 'The IUPAC Division VIII Webboard'

(2) Minute 6.3. Replace the last sentence with the following:

> 'Debate about the element names in question might have been avoided if there had been footnotes in the 'Revised 'Red Book' to explain what was done in the Tables, but the editors of the 'Revised Red Book' did not agree that such footnotes were appropriate.'

(3) Minute 7.1, line 27 Insert ‘Dr Alan McNaught’ after ‘administrator’

(4) Minute 7.1 lines 19-20, page 4. Change to ‘the University of California at San Francisco ‘ZINC’ database (ZINC is an acronym and is not a commercial database) (UCSF ZINC) (3.3 million structures).’

(5) Minute 7.6.4. Delete ‘in this document and the document under item 7.6.5’

(6) Minute 7.6.5. Read as follows:

‘7.6.5 Terminology and Nomenclature of Macromolecules with Cyclic Structures (2000-082-1-800); Task Group Leader: W. Mormann

Dr Hellwich gave a rough overview of the scope of this document. He noted noted that there is still a problem of consistency with general terms in this document and the document under 7.6.4.

The subject is completed subject to approval by the task groups at this meeting.’

(7) Minute 8.3, line 7. Change ‘structure’ to ‘formula’.

(8) Minute 8.6.3. Read as follows:

‘8.6.3 Ambiguity in Names.

It was noted that there was a meeting at 4:00 p.m. today (August 14) in Hall 10 in the Beijing International Convention Center to discuss ambiguous terminology hindering trade. Dr K.-H. Hellwich attended. The meeting dealt with analytical terminology, in particular classification of traces of pollutants, i.e., purity of products. Similar problems may well occur with improper or ambiguous chemical names (see also minute 8.6.4)’

(9) Minute 9.2 Read first sentence as follows:

‘National Representatives 2006-2007. The current number of National Representatives is 9; we are allowed 10 for this biennium according to the special modification of the Division Rules (see Appendix IV) approved for the Budapest meeting (see minute 20.1 in the Budapest meeting).’

(10) Minute 14.0 and following should be corrected to 15.0, 15.1-15.5, and minute 15.0 should be 16.0

(11) Minute 15.5 (corrected): Add the following:

‘There was discussion concerning the double Titular membership of Dr Damhaus in Division VIII and ICTNS.’

(12) Appendix III. Following Dr Jeffery Wilson, change ‘Systems’ to ‘Service

(13) Appendix IV. In the heading, the date should be (8/13/05)

(14) Appendix VII. Third entry from end: Add the name ‘Kathrin-Maria Rov’

The fully corrected minutes of the 2005 meeting of the Division Committee in Beijing are given as Appendix I. They will be submitted to Dr F. Meyers for posting on the IUPAC web site.

5.0 Matters arising from the Beijing minutes

As an example of publications by national organizations, Dr McNaught circulated a copy of the book "Signs, Symbols, and Systematics", published by the UK Association for Science Education in 2000.

6.0 Report of JCBN meeting in Bonn, May 13-14, 2006

Dr Moss and Dr McNaught reported on the meeting of JCBN held on May 13-14, 2005 in Bonn, Germany. A copy of the minutes is given in APPENDIX II. The following points were stressed.

6.1 A revision of "Nomenclature of Phosphorus-containing Compounds of Biochemical Importance, Recommendations 1976" is being formulated as a new project.

6.2 A document containing amendments to the existing "Nomenclature of Carbohydrates" is underway.

6.3 A proposal to unify the method of citation of substituents on nitrogen atoms in amino acids with that of carbohydrates is under discussion. Substitution of nitrogen atoms would be indicated by an on-line number preceding the italic letter *N* paralleling carbohydrate substitution on oxygen atoms, i.e. 2-*O*. Dr Hellwich reiterated his objection to this proposal on the basis that it conflicts with general organic nomenclature. Mr Brecher claimed that N^6-acetyllysine was less likely to cause problems than 6-*N*-acetyllysine and that the superscript system was more resilient than the carbohydrate system.

It was noted by Mr Brecher that, in his experience, the hyphenated format was more error prone.

The general feeling was that a very good case for a change to the carbohydrate system for *N*-substituents of amino acids must be made before Division VIII could agree to such a change. In addition, to recommend such a change would make search procedures more difficult because both forms would need to be included.

7.0 Publications since the 2005 meeting in Beijing

7.1 The new edition of the "Nomenclature of Inorganic Chemistry" (the Red Book), Recommendations 2005, has been published by RSC publishing; it is priced at 50.00 GBP. Dr. Hellwich has written a review, for which see: "Mehr Systematik" in: *Nachr. Chem.*, 54(7/8), 807-808, 2006.

The authors received a few comments, one regarding the inconsistency in names derived from element names, for example, anionic iron as ferride but anionic antimony as antimonide; and another an inquiry about acid names.

Comments included: The advertising by RSC was disappointing. It was noted that publishers tend to advertise what they expect to sell well. A question was raised about what is in the contract with RSC about advertising. Perhaps the Publications Committee should look into advertising by the Secretariat. Dr Moss will investigate.

7.2 A German translation of "Phane Nomenclature Part I. Phane Parent Names (IUPAC Recommendations 1998" has been published in *Angewante Chemie*, 118(23), 3967-3984, 2006.

7.3 A German translation of "Phane Nomenclature Part II. Modification of the Degree of Hydrogenation and Substitution Derivatives of Phane Parent Hydrides (IUPAC Recommendations 2002" has been published in *Angewante Chemie*, 118 (35), 6023-6033, 2006.

7.4 An Exercise Workbook on Stereochemistry in German by Dr Hellwich has been translated into English.

7.5 A general article describing InChI: "Chemical 'Naming' Method Unveiled, Free Software Converts Structures to Computable-Readable Representations", *Chem. Eng. News*, 83(34), 39-40, 2005.

8.0 Division VIII Projects

8.1 IUPAC International Chemical Identifier (InChI) (2000-025-1-800). Dr McNaught and Dr Heller reported on the InChI project as recorded in APPENDIX III. A list of presentations by Steve Heller since August 2005 and a list of InChI takeups by software developers and database providers are also given there.

Two projects proposals, one for an extension and one for the creation of an IUPAC InChI fellowship have been combined into one proposal "IUPAC International Chemical Identifier (InChI): Extension of Protocol 1.0 (2006-001-1-800)

8.2 Preferred Names in the Nomenclature of Organic Chemistry (2001-043-1-800). Dr Powell reported the status of the P-names project as follows.

8.2.1 Consideration of comments and revision of the public review draft (September, 2004) of the revised "Nomenclature of Organic Chemistry" continues. This is a very difficult process and involves constantly shifting views while trying to accommodate as many of the different opinions of reviewers as possible. It appears that Chapters 2, 3, and P-40-43 of Chapter 4 have been revised and edited. Questions are still evident about the distribution of material between Chapters 1 and 5. Chapters 6, 7, 8, 9, and 10 have been revised by Prof Favre, but not fully reviewed or edited. Appendix 1 ('a' prefixes) has been revised; Appendix 2 (substituent groups) will be revised while editing Chapters 6-10; and a new Appendix is planned summarizing the status of retained names. Prof Favre has estimated that the book should be completely edited by September, 2007. However, this will depend on many factors.

8.2.2 Several documents were distributed to Committee members for their review and comment, namely: (1) a new subsection, P-31.1.3.2 dealing with naming cyclic cumulenes; (2) a revision of P-16.3.2 covering 'bis-' vs, 'di-' and P-16.4.1 on enclosing marks, both in response to comments; (3) comments from Prof. Favre on material from P-16.3, P-16.4.1, and P-13.5.2; (4) an example needing for multiple *N* locants comparing on-line numbers with superscript numbers along with arguments for the latter from Dr Hellwich; (5) a proposed outline for revising the current P-44.

8.2.3 Concern was expressed about the slow progress in completing the project (it was scheduled to be finished in 2003. Dr Powell responded that the slow progress could be attributed to the fact that because of only two working group members, often disagreements are difficult to resolve. It was suggested that revised subsections should be posted on the webboard so as to gain input from a number of sources.

8.2.4 Dr McNaught noted that the 'Executive Committee', consisting of the President, Past President, and the Secretary, had met earlier and had suggested that the President, Dr Moss, be constituted as an administrator of the project. This proposal was supported by the Division Committee members. Dr Moss was to convey this decision to Dr Favre. Dr Powell suggested that Dr McNaught should continue as an ex-officio member of the working group.

8.2.5 P-14.7 Adducts. This new section was drafted recommending a space at each end of the 'em' dash between the names of components. This was done because of a fear that an 'em' dash might be through to be a misstyped hyphen. After some discussion the sense of the Committee was that such spaces were not necessary.

8.2.6 P-44. The Committee in general agreed with the proposed outline for dividing this subsection into two parts, P-44 becoming "Seniority order for parent structures" and P-45 as "Selection of Preferred IUPAC Names". This parallels the CAS procedure and emphasised that there can only be one parent structure in a compound on which several names can be based. It was also agreed that selection criteria dealing with nonstandard bonding numbers should be included as selection criteria for parent hydrides, but that selection criteria involving isotopic labeling and stereochemical configuration should be considered separately following other criteria for selection of preferred IUPAC names.

8.3 Rotaxanes (2002-007-1-800). Dr Yerin reported that the document "Nomenclature of Rotaxanes" has been submitted for review and the working group is awaiting comments. It was noted that since each of the component of the rotaxane name have their own separate set of locants, the addition of enclosing marks for the complete name might result in a series of enclosing marks that do not coincide with the nesting order for enclosing marks. An explanation should be included or a rule added to define the enclosing marks to be used. A suggestion to use angle brackets (</>) did not find favor.

8.4 Extension of IUPAC Rules of Stereodescriptors to Coordination Numbers 7-12 (2003-025-1). Prof Leigh reported that a Technical Report based on the final report of the project "Representation of Coordination Polyhedra and the Extension of Current Methodology" submitted last year in Beijing (see minute 7.5 of the minutes of the Division Committee in Beijing). It is to follow the normal review process for Technical Reports.

8.5 Macromolecular projects

8.5.1 Source-Based Nomenclature of Single-Strand Organic Polymers (2003-042-1-800). Prof Jones submitted the following report based on the minutes of the meeting of the Division IV Subcommittee of Polymer Terminology held in Rio de Janeiro, July 11-14, 2006.

The title of the project was changed from *Linear Polymers* to *Single Strand Polymers*. After long discussions that occur periodically on this subject it was stated that names should be used according to the presently recommended organic nomenclature whenever possible. It was also (again) stated that this is not always possible in the nomenclature systems for polymers (*e.g.*, sometimes additional adjectives or notes are required). "Deeply incorrect" although still frequently used names should be explicitly and strongly discouraged. Therefore, a list of not recommended but still allowed trivial names should be provided. Dr. Kahovec volunteered to deal with this task. In principle user-friendly names should remain allowed as far as possible and there should be guidelines for the limited use of trivial names within the proposed source-based nomenclature of single strand polymers/copolymers. Everybody was encouraged to submit corresponding comments and proposals to Prof Kitayama not later than by the end of September so that a revised draft can be prepared by the end of this year.

8.5.2 Nomenclature and Graphic Representations for Chemically Modified Polymers 1999-051-1-800 (2006-006-1-400). Prof Jones submitted the following report based on the minutes of the meeting of the Division IV Subcommittee of Polymer Terminology held in Rio de Janeiro, July 11-14, 2006.

A list of 9 points of discussion had been distributed and discussed by the Working Group and agreement on the individual items has been achieved such that a revised version can be provided for the Working Group by the end of September and a new draft presented to the Subcommittee by March 2007. It was noted that the document has made good progress since the Beijing meeting for which the Working Group leader is to be complimented.

Division IV contributed $4000 for an extension to the project. It is now a Division VIII project and it should be funded by Division VIII.

8.5.3 Nomenclature for (Macromolecular) Rotaxanes. Dr Yerin noted that this project is still on hold pending the completion of the document "Nomenclature of Rotaxanes (2002-007-1-800), for which see minute 8.3.

8.5.4 Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers (2000-081-1-800). Dr Kahovec noted that a draft was completed several years ago but several problems still need to be resolved. It was divided into two parts, one dealing with dendritic polymers and a second with hyperbranched polymers. The funding ran out in 2002. An application for an extension was submitted in 2003.

8.5.5 Structure-Based Nomenclature for Cyclic Macromolecules (2001-082-1-800, extension 2004-046-1-800). Dr Hellwich submitted the following report on this project formerly called "Terminology and Nomenclature of Macromolecules with Cyclic Structures".

After the meeting in Beijing 2005 during which a few proposals were made, a new Draft was prepared by Prof W. Mormann and Dr K.-H. Hellwich which was sent to the members of the Subcommittee on Macromolecular Terminology on August 24, 2005; comments were received by Dr Ted Wilks. Thereafter the document was sent (on September 29, 2005) to 12 experts, five of which responded. Comments were discussed in a meeting of Prof Mormann and Dr Hellwich on February 28, 2006 in Altenstadt, Germany. Those comments which were appropriate have then been incorporated into a new draft. In detail the following changes were made:

1. The definition of "cyclic macromolecule" (CM-1.7) has been changed and a note has been added to the definition of "macrocycle" (CM-1.9).
2. The proposal of using "pluricyclic" instead of "polycyclic" was discussed. The decision was not to adopt this proposal. A corresponding note has been added.
3. Also the suggestion for a unified orientation of formulae, i.e. to generally place the subunit of highest seniority in its upper left part and proceed clockwise with naming, has been dealt with in an additional note to example 8.
4. A proposal by Prof Tezuka to change the nomenclature in such a way that the user can easily recognise the overall topology from the name was refused after a short discussion because this is, in general, not possible in structure-based nomenclature. A paragraph has been added in the introduction explaining that topology is not an explicit topic in structure-based nomenclature, although it is inherently contained in a structure-based name, and giving reference to publications on topology by Prof Tezuka.

This revised draft reflecting the comments of the experts was then sent to Prof Jones on March 7, 2006. Comments by him (linguistic, formal and content-related) were received on April 10, 2006 and dealt with in a further meeting of Prof W. Mormann and Dr K.-H. Hellwich on June 12, 2006 in Siegen, Germany. The major resulting change is the addition of the three definitions of "spiro compound", "spiro macromolecule" and "spiro union" (CM-1.16 to CM-1.18) to the glossary. No further comments on this new draft have been obtained during the meeting of the Subcommittee on Macromolecular Terminology in Rio de Janeiro (July 11 – 14, 2006). The document is therefore ready for ICTNS and Public Review.

8.6 Cyclic Peptides (2004-024-1-800). Dr Moss reported that there has been little progress in moving this document forward from its public and IDTNS review stage. It was mentioned that the method used by CAS should be incorporated.

8.7 Graphical representation standards (2003-045-1-800). Mr Jonathan Brecher provided the following report on the status of projects dealing with graphical representation of chemical structures.

8.7.1 The report "Graphical Representation of Stereochemical Configuration (IUPAC Recommendations 2006)" will appear in the October issue of PAC.

8.7.2 A revised draft of "Graphical Representation Standards for Chemical Structure Diagrams (IUPAC Recommendations 2007) was discussed at the Project Groups meeting here in Prague. It should be ready for the review process by the end of the year (2006).

8.7.3 The question of whether to include recommendations for drawing macromolecular structures was raised. This could be a reason for extending the basic project. The existing macromolecular document does need to be revised.

8.8 Nomenclature of phosphorus containing compounds of biochemical importance (2006-019-1-800). As noted above in minute 6.1 this project was only recently approved as a project. A draft is almost ready for review.

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

The document entitled "A Comparison of Nondetachable Hydro Prefixes (IUPAC), Added Hydrogen (CAS), and Indicated Hydrogen (Beilstein), in Expressing Substitutive Suffixes" prepared several years ago as recommendations by the IUPAC Commission on Nomenclature of Organic Chemistry, but currently planned as a technical report was sent to Dr Wilson and Dr Hellwich for a final check of the CAS and 'Beilstein' names that are cited.

Dr Hellwich suggested that the approach currently recommended in the new revised Blue Book be added. This has been done. However, this could affect publication as a technical report, since new material is now present which will precede publication of the revised Blue Book. The revised document will be sent to Prof Herold, Secretary of IDTNS, for evaluation and a recommendation.

9.0 Future Projects

9.1 2nd edition of *Principles and Practices of Chemical Nomenclature, A Guide to IUPAC Recommendations* , 1998. Dr Leigh prepared a project proposal which was reviewed and revised to reduce the total cost. Project meetings are planned for January, 2007; August, 2007; August, 2008; and a final meeting in January, 2009. It was noted that the new revised Blue Book and the several macromolecular documents need to be closer to completion.

9.2 Preferred names for inorganic compounds Prof Hartshorn reported that a meeting of a project team was held in Copenhagen, Denmark on April 12-13, 2006. The minutes of

this meeting are given as APPENDIX IV. As a result of this meeting, a project proposal was developed and submitted for review.

9.3 Preferred structure-based names for macromolecules. Prof Jones reported that there has been no mention of such a project in the Subcommittee on Macromolecular Terminology in Division IV. However, it would appear that the main requirement of such a project would be to use PIN names for constitutional repeating units. Prof Jones and Dr Kahovec will discuss this matter here in Prague.

9.4 Metallacycles. Prof Hutton reported that one of the topics that came up during the meeting for the inorganic PINs project in Copenhagen (see minute 9.2 above) was the oft-proposed project on "Nomenclature of Metallacycles". Minute 8.2 of the Beijing minutes noted that Dr McNaught was to write to Prof Kaesz to determine the status of the project. Dr McNaught reported that no reply came from Prof Kaesz. Dr Powell had put together a draft project proposal, but nothing further has been done. Version 2 (a revised version of version 1.5) of a draft entitled "Nomenclature of Metallacycles of the Transition Metals" dated June 25, 2001 authored by Prof Kaesz, Dr James Casey, Prof Favre, and Prof Yamamoto. Dr Powell and Prof Hutton have discussed this matter here in Prague and Prof Hutton agreed to prepare a new draft project proposal.

9.5. Boron nomenclature. Dr McNaught has been attempting to get someone interested in leading such a project. Interest had been expressed from members of the organizing committee of the International Boron Symposia and there was correspondence with several potential participants in a nomenclature project, but when it became apparent how much work might be involved, interest rapidly declined.

9.6 Other projects

9.6.1 Interest has been expressed in a project on inorganic polymers, essentially a revision of Chapter II.7 (Regular Single-strand and Quasi Single-strand Inorganic and Coordination Polymers) of Red Book II.

9.6.2 Nomenclature of calixerenes. This was originally included in a broad project along with rotaxanes.

9.6.3 A single book on stereochemistry, which was a former project of organic stereochemistry has been subsumed into Chapter 9 of the revised Blue Book.

10.0 Membership

10.1 The Committee paused to honor Prof J. Rigaudy, Titular member of the Commission on Nomenclature of Organic Chemistry from 1967-1981 and its Chairman 1977-1981, who died in December, 2005. Prof Rigaudy was largely responsible for the development of the nomenclature for isotopically modified organic compounds and instrumental in the early preparation of the 1993 Guide to the Nomenclature of Organic Compounds.

10.2 The membership of the Committee was evaluated in preparation for elections in 2007. The terms of five regular Titular members will expire, but all can be renewed: Dr Damhaus, Prof Hartshorn, Dr Kahovec, Prof Nytrai, and Dr Yerin. Dr McNaught's term as Past-President will expire and Dr Powell will resign as Secretary in 2007.

There are no Associate Members terms expiring in 2007.

Because there will not be a Past-President after 2007, a Vice-President should be elected in order to have an Executive Committee with three Officers.

10.3 Nominating Committee. By Division Rules, the nominating committee consists of five members with no more than two members from the existing Division Committee and the other three chosen from outside IUPAC on the basis of the breadth of their expertise. The Division President will not be a member of the Nominating Committee. The names Prof Jim Bull, Dr David Martinson, and Prof Robert Stepto were suggested as the three NON-Division members of the Nomenating Committee with Prof Jim Bull as Chairman. Dr McNaught and Dr Kahovec were suggested as Division members.

10.4 Several suggestions for consideration by the Nominating Committee were put forward. Dr Damhus was suggested.as a potential candidate for Secretary. Prof J Reediyk, Prof Kitayama, and Prof Nordlander were suggested as potential members of the Division Committee.

10.5 National Representatives. All must be renewed or replaced every two years.

10.6 Advisory Subcommittee. The membership should be reviewed every two years. Between now and the meeting in Turin, each member should be asked whether or not they are still interested in serving on the Subcommittee.

Past members of the Division Committee should be included on the Subcommittee, if it is their desire to do so. Members of the Division IV subcommittee on Macromolecular Terminology should be approached regarding membership on the Division VIII Advisory Subcommittee. Are there persons with interests in biochemistry, for example, Dr Marcus Ennis and Dr Kiril Degtyarenko that would serve as members of the Advisory Subcommittee?

10.7 We need to be always on the lookout for persons interested in nomenclature. National Adhering Organizations should be encouraged to suggest names for any type of membership; these names should be passed on to the Nominating Committee. The Advisory Subcommittee should be asked for suggestions for membership at any level.

11.0 Election procedures. Prof Leigh renewed his recommendation to have a broader base for elections. Members of the Advisory Subcommittee should be involved.

12.0 Publicity

12.1 Projects must have a plan for publicizing their outcome. The InChI project is a good example. Dr Heller gives talks around the world (see minute 8.1 and Appendix II).

12.2 Book Reviews (see book review by Dr Hellwich, minute 7.1). The main question raised here is who has the responsibility to send books to reviewers.

12.3. There is a section in CI called “Up for discussion” that can provide a place for short articles promoting Division VIII activities or discussing nomenclature questions and problems. See, for example, the article “What is Butadiene?” by Dr Hellwich in the March/April 2006 issue, which notes the importance for authors to be precise in their nomenclature.

12.4 Translations:

12.4.1 German translations. Since 2002 the journal *Angewandte Chemie* (*Angew. Chem.*) has been publishing translations of IUPAC Recommendations and Technical Reports into German.

Four translations appeared in 2005 (For translations published earlier, see Appendix VII to the minutes of the Beijing Division Committee meeting).

Gerrit Schüürmann
Modellierung der Lebensdauer und Abbaubarkeit organischer Verbindungen in Luft, Boden und Wasser, *Angew. Chem.* **2005**, *117, Nr. 5*, 834 – 845
Original: *Pure Appl. Chem.* **73**, 1331 – 1348 (2001)

Dietmar Schomburg
Nomenklatur der Lignane und Neolignane, *Angew. Chem.* **2005**, *117, Nr. 15*, 2339 – 2351; **2006**, *118, Nr. 23*, 3983
Original: *Pure Appl. Chem.* **72**, 1493 – 1523 (2000)

Carlo Thilgen
Nomenklatur der Fullerene C_{60}-I_h und C_{70}-$D_{5h(6)}$, *Angew. Chem.* **2005**, *117, Nr. 31*, 5065 – 5108
Original: *Pure Appl. Chem.* **74**, 629 – 695 (2002)

Hans Schick,* Karl-Heinz Hellwich,* Kathrin-Maria Roy
Überarbeiteter Abschnitt F: Naturstoffe und verwandte Verbindungen, *Angew. Chem.* **2005**, *117, Nr. 47,* 7985 – 8014; Erratum: **2006**, *118, Nr. 23*, 3983
Original: *Pure Appl. Chem.* **71**, 587 – 643 (1999); **76**, 1283 – 1292 (2004)

By the end of 2006 four further translations will have been published, three sets of recommendations and one technical report. Note the new German term for Phane Nomenclature (Phannomenklatur)

Werner Steck,* Karl Cammann
Harmonisierter Leitfaden für die Validierung von Analysenmethoden durch Einzellaboratorien, *Angew. Chem.* **2006**, *118, Nr. 12*, 2019 – 2034
Original: *Pure Appl. Chem.* **74**, 835 – 855 (2002)

Karl-Heinz Hellwich*
Phannomenklatur Teil I: Phanstammnamen, *Angew. Chem.* **2006**, *118, Nr. 23*, 3967 – 3984
Original: *Pure Appl. Chem.* **70**, 1513 – 1545 (1998)

Karl-Heinz Hellwich,* Kerstin Ibrom
Phannomenklatur Teil II: Änderung des Hydrierungsgrades und Substitutionsderivate von Phanstammverbindungen, *Angew. Chem.* **2006**, 118 (35), 6023-6033, 2006.
Original: *Pure Appl. Chem.* **74**, 809 – 834 (2002)

Heiko Leuken
A Technical Report: Praktische Anleitung zur Messung und Interpretation magnetischer Eigenschaften, A*ngew. Chem*. **2006**, *118, Nr. 47*, 8233 – 8240.
Original: *Pure Appl. Chem*. **2005**, 77, 497-511

12.4.2 We should write to National Adhering Organizations to encourage translations of IUPAC documents.

12.5 IUPAC and IUBMB nomenclature web site. Dr. Moss distributed statistics on his web site and Queen Mary College. They are reproduced in APPENDIX V.

12.6 IUPAC web site. The Division VIII webboard on the RSC site will be maintained until the new IUPAC webboard site is operational.

13.0 Reports from other committees

13.1 Committee on Chemistry Education (CCE). This Committee coordinates the educational activities of IUPAC and monitors educational activities throughout the world.

Prof Hartshorn reported that the Committee met in Seoul, South Korea in early August, but that he had not been able to attend and minutes of that meeting had yet to be circulated. Ideas for Division VIII projects of interest to CCE might include a tutorial on graphical representation of chemical structures. It would be valuable to know exactly who CCE communicates with. This might be an avenue for publicity for Division VIII activities.

13.2 Committee on Printed and Electronic Publications (CPEP). Dr Heller reported on the meeting of CPEP in Berlin, in July, 2006 as follows:

13.2.1 The transfer of the IUPAC web site server from a commercial provider to FIZ CHEMIE Berlin, is the sole responsibility of the IUPAC task force. This transfer went so smoothly that the CPEP committee especially gave thanks to the colleagues in Prague who did the work; the group of Bohumir Valter, Mila Nic and Beda Kosata who organized the transfer. The committee also expressed its appreciation to FIZ CHEMIE Berlin who provided the hardware and will maintain the system.

The IUPAC website appears to be for use by IUPAC members and not for the general public. The URLs of current pdf files will not change. Dr. Moss reiterated that we should be sure that statistics like he keeps can be obtained from the IUPAC website.

13.2.2. For future web site plans it was decided to improve the tool kits and the navigational functions of the IUPAC server and as well bit by bit to include all IUPAC relevant sites. CPEP, along with David Black (IUPAC Secretary General) again indicated it was unhappy that the transfer of IUPAC content from the Gerry Moss web site was not yet implemented. It was noted that Dr Black had not approached Dr Moss about this matter.

13.2.3. The policy of mirror sides will be kept, to insure that the content of this server can be read without problems, everywhere on this world.

Questions about monitoring and checking the results of updating mirror sites were mentioned. Is CPEP or the Secretariat to oversee the content? The CPEP's Chairman. should be contacted about these question.

13.2.4. Another topic of interest that was discussed is the standardization of multimedia or teaching materials for long-term preservation.

13.2.5. The current and future developments of the InChI - International Chemical Identifier - was discussed, including the possibility of extended InChI to handle chemical reactions. All CPEP members expressed their pleasure as the rapid rate of adoption of InChI by the commercial, government, and academic world.

13.2.6. An ad-hoc committee of 5-6 people, at the request of the IUPAC President, is being established by the Secretary General to look into the issue of how databases can best be established and disseminated via the IUPAC web site and other mechanisms. This committee was created as a result of numerous Division presidents indicating the need for such an effort, citing the atmospheric chemistry, solubility, and stability constants databases as two examples that need to be examined. It was felt that input from database user groups like the Analytical and Physical Divisions was very much needed at this time.

Division VIII is not really involved with this issue, since it does not deal with databases.

13.2.7 Comments included a request for CPEP to discuss the issue of advertising with respect to the new edition of the Red Book and future book revisions. We, Division VIII must decide what we expect from CPEP or from RSC about book publishing, and what is our responsibility.

13.3 Committee on Chemistry and Industry (COCI). COCI is the focus for issues of importance to the global chemical industry. Dr McNaught noted that the most recent meeting was held in Chicago, July 20-21, 2006.

13.4 PAC Editorial Advisory Board. The inaugural meeting of the reconstituted PAC Editorial Advisory Board (suspended since 1999) was held August 19, 2005 in Beijing. Dr McNaught noted that there was nothing of importance to Division VIII to report at this time.

Based on his experience with publication of the graphical configuration paper, Mr Brecher expressed his displeasure with the publication process. It took six months for this document to go through the process and was out for review three different times.

Dr Powell noted a similar experience with the paper on numbering of fullerenes.

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

The purpose of ICTNS is to maintain quality of IUPAC recommendations with respect to nomenclature and symbols. Dr McNaught noted that ICTNS has three members from Division VIII to represent nomenclature matters, Dr McNaught, Dr Damhus, and Prof Nyitrai who represents Division VIII. Dr J. Kahovec represents Division IV.

14.0 Other business

14.1 Dr Garnot Eller sent to us a manuscript entitled "Improving the Quality of Published Chemical Names with Nomenclature Software" for consideration as a publication. Discussion indicated that it should not be published as a PAC article. It was suggested that a two page article in CI with web backup with results. Dr Moss will write to Dr Eller.

14.2 A call from Dr Herve Schepers of the European Union asking for scientific and technical assistance for Scientific Customs. It was agreed that this was not something that Division VIII could become involved with, but his request could be circulated to individual members and the Advisory Subcommittee.

14.3. Dr Hellwich asked for advice on how to deal with requests for IUPAC names that he receives. In answer, it was noted that IUPAC (Division VIII) has no obligation to respond. For the future, the Secretariat should be asked how to deal with questions directed to Division VIII on the IUPAC website.

14.4 Difference between rule and recommendations. Recommendations better reflect the status of IUAC rules and are without any power of enforcement.

15.0 Future meetings: The next meeting of the Division Committee will be at the General Assembly in Turin, Italy, August 4-12. There are no current plans for a meeting in 2008. In 2009, the General Assembly will be in Glasgow, Scotland, August 1-9.

Respectfully submitted: Warren H. Powell, Secretary, January 3, 2007

Approved: Gerald P. Moss, President, January 10, 2007

APPENDIX I

Minutes of the IUPAC Chemical Nomenclature and Structure Representation Division (VIII) Committee Meeting

Beijing, China, August 13-14, 2005

Members present: Mr Jonathan Brecher, Dr Ture Damhus, Prof Richard Hartshorn, Dr Stephen Heller, Dr Michael Hess**,** Dr Jaroslav Kahovec, Prof G Jeffery Leigh**,** Dr Alan McNaught (President), Dr Gerard Moss, Prof József Nyitrai, Dr Warren Powell (Secretary), Dr Matthew Toussant, Dr Andrey Yerin

Representatives from other IUPAC bodies present: Prof David StC Black (IUPAC Secretary General)

National Representatives Present: Prof Jan Reedijk (Netherlands), Dr Paolo Righi (Italy)

Observers: Dr David Barden (RSC Young Observer), Dr Karl-Heinz Hellwich (elected Titular Member for 2006), Dr William Town, in part (Project Leader, Graphical Representation Standards)

Members Absent (excused): Prof Herbert Kaesz, Prof Dr Alexander J. Lawson, Dr Antony Williams

The fifth meeting of the Division Committee of the IUPAC Division of Chemical Nomenclature and Structure Representation at the Beijing International Convention Center was convened by President McNaught at 9:00 a.m. on Saturday, August 13, 2005.

1.0 President McNaught welcomed the members to this meeting and offered a special welcome to the National Representatives, Prof Jan Reedijk (Netherlands) and Dr Paolo Righi (Italy): to Dr David Barden, a Young Observer from the Royal Society of Chemistry; and to Dr Karl-Heinz Hellwich, an elected Titular Member for 2006. He also noted that Prof Herbert Kaesz, Prof Dr Alexander J. Lawson, and Dr Antony Williams would be unable to be with us. It was noted that Prof David Black, the IUPAC Secretary General, would be visiting during the meetings and that Dr Peter Atkins, Chairman of the IUPAC Committee on Chemical Education, would join our meeting at some point. Each of the attendees introduced himself and provided some background information. Housekeeping details regarding breaks and lunch were announced.

2.0 The agenda as circulated was approved with the addition of the following topics:

Cross representation on other international bodies (minute 13.0).
Elections (minute 9.5)
Translations of IUPAC recommendations (minute 14.0)
The IUPAC Division VIII Webboard (hosted by RSC) (minute 13.2)

3.0 The minutes of the Division Committee Meeting in Budapest, Hungary on August 30-31, 2004 as posted at:

http://www.rsc.org/IUPAC8/attachments/DivisionCommitteeMinutesBudapestFinal.rtf

http://www.rsc.org/IUPAC8/attachments/DivisionCommitteeMinutesBudapestFinal.pdf

were approved with the following correction.

3.1 Item 7.3 (2) should read “Dr Damhus submitted examples to try to coordinate the use of the multiplicative prefixes 'di, tri, ...' vs. 'bis, tris, ...' between the revised Blue Book and the soon to be published Red Book.

4.0. Matters arising from the Budapest minutes.

4.1. It was noted that the document ‘Graphical Representation of Stereochemical Configuration’ uses ‘not acceptable’ rather than ‘unacceptable’ as given in item 17.0 of the Budapest minutes. It was agreed that this usage should be retained.

5.0. Report from the meeting of the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) in Columbia, Missouri on April 30th and May 1st 2005.

The minutes of the meeting of the Nomenclature Committee of IUBMB (NC-IUBMB) and the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) held in Columbia, MO, USA on April 30-May 1, 2005 may be found at:

Dr Moss noted that the meeting in Columbia, MO was concerned mostly with enzymes.

Dr McNaught reported that the enzyme information database BRENDA now uses InChI.

Developing projects in IUPAC-IUBMB that will require IUPAC approval:

(1) An addendum to the 1996 carbohydrate nomenclature, to include areas not well covered in that document.

(2) A revision of the old JCBN document on Phosphorus-Containing Compounds of Biochemical Importance (*Eur. J. Biochem.* **1977**, *79*, 1-9; Biochemical Nomenclature and Related Documents, 1992, pp. 256-265)

(3) Compilation of a list of biochemical compounds that are not a part of any other IUPAC-IUBMB documents and for which advice is needed.

Membership: Prof Dietmar Schomburg was appointed as Chairman (funded by IUBMB) and Prof Sinéad Boyce reappointed as Secretary (funded by IUBMB). Prof Richard Cammack will serve as Past Chairman and Treasurer. Prof J. F. G. Vliegenthart (IUBMB) and Dr Gerry Moss (IUPAC) were reappointed to four-year terms. The Division VIII Committee endorsed these appointments.

6.0 Publications since the 2004 meeting in Budapest:

6.1 Numbering of Fullerenes, *Pure Appl. Chem*, **2005**, ***77***, 801-923:

There were 200 reprints of this publication sent to Dr Powell. This seems far to many in this age when copies are so readily available on line. This needs to be discussed by the Publications Committee.

6.2 "International chemical identifier goes online", *Chem. World*, **2005**, ***6***, 7:

6.3 In the July-August issue of *Chem. Int.* there is an article about the treatment of element names in the new edition of the "Red Book" by P. Goya and P. Román specifically titled "Wolfram vs. Tungsten", along with a reply from Dr Ture Damhus on behalf of the editors of the 2005 "Red Book". This may be found at:

http://www.iupac.org/publications/ci/2005/2704/ud_goya.html

It was noted that there are numerous differences in naming and/or spelling of element names for nationalities other than English. Debate about the element names in question might have been avoided if there had been footnotes in the 'Revised 'Red Book' to explain what was done in the Tables, but the editors of the 'Revised Red Book' did not agree that such footnotes were appropriate.

7.0 Division VIII Projects:

7.1 IUPAC International Chemical Identifier (InChI) (Dr Steve Heller)

The IUPAC International Chemical Identifier (InChI) is a protocol for converting a chemical structure (connection table) to a unique, predictable ASCII character string. Version 1.0 of the Identifier released in April 2005 expresses chemical structures in a standard machine-readable format, in terms of atomic connectivity, tautomeric state, isotopes, stereochemistry, and electronic charge. It deals with neutral and ionic well-defined, covalently-bonded organic molecules, and also with inorganic, organometallic and coordination compounds. Software, documentation, source code, and licensing conditions are available from the IUPAC website at:

http://www.iupac.org/inchi

An InChI frequently asked questions (FAQ) by Nick Day (Unilever Centre for Molecular Informatics, Cambridge University) is available from:

http://wwmm.ch.cam.ac.uk/inchifaq/

A full publication of the InChI protocol probably will appear in a NIST journal within the next year.

A new project, titled "IUPAC International Chemical Identifier (InChI) Promotion and Extension (2004-039-1-800)" has been established to promote the use of the Identifier throughout the chemical information community; to extend its applicability to include polymeric structures; to explore the need for other extensions, including the ability to handle Markush structures; and to include information on other attributes, such as phases and excited states. For additional information see:

http://www.iupac.org/projects/2004/2004-039-1-800.html
http://webboard.rsc.org:8088/~INCHI-L

It was suggested that InChI be publicized outside of information circles.

To enable development of InChI facilities and applications in an Open Source context, a project to encompass this work has been registered with SourceForge.net

(see http://sourceforge.net/projects/inchi); anyone wishing to participate should contact the project administrator, Dr Alan McNaught (mcnaughta@rsc.org) or the IUPAC Secretariat (secretariat@iupac.org). To receive and discuss proposals for InChI enhancements, an Internet listserver has also been established; anyone wishing to participate in these discussions should contact Dr Alan McNaught (mcnaughta@rsc.org).

There are two problems that must be recognized. One is related to chemistry, i.e., how the structure is drawn, for example, tautomers. The other is interpretation by the chemist. An InChI cannot be derived if the structure cannot be accurately drawn or can be represented as a molfile; InChI is based on molfile. InChI must support many formats, included disconnected diagrams. It is necessary to be able to verify that the output from an InChI is the same as the input.

Although in principle publishers could probably derive InChIs more easily than authors, publishers may not be willing to take on the extra work and may leave the responsibility for InChI generation to the authors.

In May, 2005, ACD Labs announced that they would be fully implementing the InChI protocol into their structure drawing program ACD/ChemSketch. U.S. Patent Office is interested in InChI. The European Patent Office expressed interest one and a half years ago, but nothing has developed yet.

CAS is looking into various formats and doesn't see InChI being used in its products today. Beilstein is considering InChI and seems to like it, but management has yet to be convinced.

InChI has been adopted by the National Institute of Standards and Technology (NIST)(150,000 structures); the National Institutes of Health/National Centre for Biotechnology Information (NIH/NCBI)/PubChem (3 million+ structures; the National Cancer Institute (NCI) Database (23 million+ structures; the Environmental Protection Agency Distributed Structure-Searchable Toxicity (EPA DSSTox) Database (1450 structures); the Kyoto Encyclopedia of Genes and Genomes (KEGG) Database (9584 structures); the University of California at San Francisco ZINC (ZINC is the acronym for ZINC is not a commercial database) (UCSF ZINC) (3.3 million structures).

InChIs can be searched in Google.

A list of talks about InChI given in 2005 appears in Appendix I. After they are actually given they will be available on Dr Steve Heller's website (http://www.hellers.com/steve/pub-talks/)

Appendix II gives a list of InChI references and/or publications.

7.2 Preferred names in the nomenclature of organic compounds: new Blue Book (Dr Warren Powell)

The revised "Nomenclature of Organic Chemistry", a more comprehensive set of recommendations than has ever been attempted previously and which contains recommendations for selecting preferred IUPAC names (PINs), was submitted for public and ICTNS review last fall. The deadline for comments was set at March 31,

2005. A number of comments and suggestions were submitted to the Division's Webboard before the deadline, dealing with topics such as proper use of 'di-', "tri-", etc. *vs*. "bis-", "tris-", etc: enclosing marks, amine oxides, acid esters, compound locants, adducts. Consideration of these items was started immediately, i.e., before the deadline for comments. Comprehensive sets of comments were received from U. Buenzli-Trepp, and G. Eller. Comments or other contributions were also received from G. Moss, T. Damhus, E. Godly, J. Brecher, L. Maat, J. Nyitrai, K-H. Hellwich, R. Sayle, R. Cammack, J. Wilson, A. Yerin, R. H. de Rossi, J. Reedijk, B. Herold, H. Schepers, J. Kahovec, A. Senning, H. Dixon, H. Gottlieb, L. Salvetella, M. Ennis, R. Hartshorn, and P. Mata.

Prof Favre, Dr Powell, and Dr McNaught met in Boston April 25-28, 2005 to evaluate all the comments received to date and to prepare for appropriate revisions to the September, 2004 manuscript.

At the present time, Chapter 1 has been revised (sections on multiplicative nomenclature, functional class nomenclature, and adducts are not yet incorporated) and Chapters 2, 9, and 10 have been revised. Major revisions are still to be incorporated in Chapters 3-6. Comments on Chapters 7-8 have still to be evaluated. There are enough significant revisions to the manuscript that it may be necessary to undergo further reviews. A real problem is how to do reviews of such an extensive manuscript thoroughly, but efficiently. There are few people willing to tackle the entire work. Perhaps it could be divided among several reviewers, but this raises questions of consistency between sections.

7.3 Nomenclature of inorganic chemistry: revision of the Red Book (Dr Ture Damhus)

The task group for revision of "Nomenclature of Inorganic Chemistry" (the Red Book) is waiting for a second page proof after which Prof N. Connelly will prepare the index. There will not be time to review the index as was suggested in Budapest. It was noted that the index to the 1990 edition as prepared by Blackwell Science was deemed not adequate by a number of readers. Dr Hellwich volunteered to look over the index if it would fit into his available time.

7.4 Rotaxanes (Project 2002-007-1-800; Dr Andrey Yerin)

Comments and proposals sent via e-mail by Edward Wilks and Jaroslav Kahovec were considered at a meeting of the project group in Budapest (August 2004). Since several comments complained that the document is very difficult for chemists not so experienced in nomenclature, it was decided to separate the document into two different parts: (1) general rotaxane nomenclature and (2) designation of configuration in rotaxanes. Because of this general change most topics had to be reformulated.

The next version of the document (Version D) was distributed to the project group members at the beginning of July, 2005. Approval of Version D and consideration of comments from Dr Metanomski are scheduled for the Beijing meeting of the project group on August 10, 2005, after which the document can be made available for public review.

Assuming that all main terms and procedures of rotaxane nomenclature are covered by this project, the preparation of a new draft document on Nomenclature for Macromolecular Rotaxanes is planned (see minute 7.6.3)

7.5 Extension of IUPAC rules for stereodescriptors to coordination numbers 7-12 (Project 2003-025-1; Prof G. Jeffery Leigh)

A project task group was established in Budapest to evaluate procedures for describing geometry of coordination polyhedra with coordination numbers 7 through 12. A final report of this project can be found on the Division VIII webboard under General messages.

http//www.webboard.rsc.org/IUPACVIII

A Technical Report based on this report is in preparation.

The main problem in describing the stereochemistry of coordination polyhedra is recognition of a discrete polyhedron because of distortion. This problem becomes more difficult as the number of coordination sites increases. The report recommends that IUPAC endorse the method of Dr T. E. Sloan, et. al., for all recognized coordination numbers up to and including coordination number 7 and be extended to include specific examples that are deemed reliable for coordination numbers 8 and 9.

7.6 Macromolecular projects (with Division IV)

A general progress report from Michael Hess can be found at:

The next edition of the "Compendium of Macromolecular Nomenclature" should be published next year. Dr Metanomski and Dr Wilks are giving it a final check. It is a compilation of already published material and will not be subjected to the full formal review processes. It was noted that the names in the older chapters are not in conformity with the 1993 Guide to IUPAC Nomenclature of Organic Compounds.

A feasibility study of a project on abbreviations is being considered.

7.6.1 Source-Based nomenclature of Single-Strand Organic Polymers (2003-042-1-800)
Task group Leader: T. Kitayama

This is an ongoing project.

7.6.2 Source Based Nomenclature for Modified Polymer Molecules (1999-051-1-800)
Task Group Leader: T. Kitayama

This is an ongoing project.

7.6.3 Nomenclature for (Macromolecular) Rotaxanes (2000-037-1-800)
Task Group Leader: A. Yerin

Work on the document "Nomenclature for Macromolecular Rotaxanes" was stopped at the Ottawa meeting in 2003 because of the project "Nomenclature for Rotaxanes" (2002-007-1-800) which was devised to develop general principles for nomenclature of rotaxanes not containing macromolecular units. Now that this latter project is almost finished and all main principles of rotaxane nomenclature are agreed, the work

on recommendations for nomenclature of rotaxanes containing macromolecular units can continue. All changes necessary to follow the developed principles for naming low molecular mass rotaxanes will applied.

The latest available draft of Nomenclature for Macromolecular Rotaxanes is dated 2003 and includes comments sent for the meeting of the task group in Ottawa. As all main definitions are already included in the low molecular mass rotaxanes document, the 2003 draft on macromolecular rotaxane nomenclature can be reduced and will deal only with the macromolecular parts of rotaxane nomenclature.

Discussion of the work needed to finish the recommendations for macromolecular rotaxane nomenclature is scheduled for the meeting of the rotaxane project group (2002-007-1-800) here in Beijing on August 10th 2005; consultation with Division IV is needed.

7.6.4 Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers (2000-081-1-800); Task Group Leader: J. Kahovec

The next steps will be expert review followed by public and ICTNS review. A list of reviewers is still needed.

7.6.5 Terminology and Nomenclature of Macromolecules with Cyclic Structures (2000-082-1-800); Task Group Leader: W. Mormann

Dr. Hellwich gave a rough overview of the scope of this document. He noted noted that there is still a problem of consistency with general terms in this document and the document under 7.6.4.

The subject is completed subject to approval by the task groups at this meeting.

7.7 Cyclic peptides (Dr Gerard Moss)

The document "Nomenclature of Cyclic Peptides (Recommendations, 2004)" has been through both public and ICTNS review. Several issues, mostly of a biochemical nature, need to be settled. The main problem is the use of the term 'cyclo' in a way that is not consistent with its use in natural products nomenclature. Publication will probably occur later in 2005.

7.8 Graphical representation standards for chemical structure diagrams (Dr Jonathan Brecher)

Since the meeting of the Division Committee in Budapest (2004), the comprehensive set of recommendations "Graphical Representation of Configuration" recently completed public and ICTNS review. Feedback from external reviewers and ICTNS members was very useful but did not contain fundamental criticisms. A small number of remaining issues were discussed and resolved during the meeting of the project task group here in Beijing. It is expected that these recommendations will be ready for publication very soon, once the conclusions reached by the project task group are transcribed into the final document.

The project task group has also started work on the second part of its responsibility, i.e., a document containing recommendations for all other (non-stereochemical) aspects of graphical structure representation. Significant work has been completed on that document titled "Graphical Representation Standards for Chemical Structure Diagrams"; it is already one-third longer than the document on recommendations for configuration discussed above.

Some of the remaining issues slated for inclusion in this document were discussed by the project task group in Beijing, but others remain to be considered. It is hoped that this document will be ready for public and ICTNS review during the first half of 2006.

In light of rapid progress in both of these areas, it has proven too difficult to keep the html version of the two documents syncronized with the pdf version. Accordingly, the html version that was formerly posted at angelfire.com is no longer available. The pdf version is being circulated among members of the working party periodically as changes are made, and could be provided to other interested parties if there is concern about the loss of the html version.

7.9 Comparison of procedures for naming hydro derivatives of fused ring systems (Dr Warren Powell)

As noted in minutes of the meeting of the Division Committee in Budapest (minute 7.11) the document entitled "A Comparison of Nondetachable Hydro Prefixes (IUPAC), Added Hydrogen (CAS), and Indicated Hydrogen (Beilstein), in Expressing Substitutive Suffixes" prepared several years ago as recommendations by the IUPAC Commission on Nomenclature of Organic Chemistry, but now planned as a technical report, was sent to Dr Karl-Heinz Hellwich and Dr Jeffrey Wilson for review of the respective Beilstein and CAS procedures. Their comments and corrections have been received but have not yet been incorporated into the document.

It was noted that an example reflecting this comparison should be added to the new Blue Book in an appropriate Section. It was also noted that Beilstein's AUTONOM will attempt to follow the IUPAC recommendations. However, at present Autonom favors the functional group over indicated hydrogen for numbering. Dr Hellwich will check this out.

Although not yet public, the URL for this document is:

http://www.chem.qmul.ac.uk./iupac/misc/hydro.html

8.0 Future Projects

8.1 Preferred names for inorganic compounds (Dr Ture Damhus)

A meeting of those who had expressed an interest to Dr Damhus in a project to develop preferred names for inorganic compounds was held in Budapest. The report of this meeting is given as Appendix III. Because of commitments to the revised Red Book, to ICTNS, and other projects, Dr Damhus was unable to prepare a project proposal and will not be able to lead such a project. Hence, a steering group consisting of Prof R. Hartshorn, Prof J. Reedijk, Prof J. Leigh, and Dr T. Damhus was formed to develop a proposal for work on preferred names for inorganic compounds. A place and time for a meeting was to be discussed.

8.2 Metallacycles (Warren Powell)

A project proposal is being developed by Prof. H. Kaesz and Dr W. Powell based primarily on a previous report by Prof H. Kaesz, Mr J. Casey, Prof H. Favre, and Prof Y. Yamamoto entitled "Nomenclature of Metallacycles of the Transition Metals**"** dated June 25, 2001. It was noted that Dr A. Hutton and Prof E. Nordlander should be a part of this project. The scope of the project was said to be too broad; the 'ocene' type of

compound should not be included but should be a separate project. Dr McNaught would write to Prof. H. Kaesz about this.

8.3 Adducts (Dr Warren Powell/Dr Ture Damhus)

In response to requests mainly from the project group for the revised Red Book, consideration has been given to adding a subsection to the new Blue Book to deal with addition compounds, other than those involving boron compounds as given in Section P-68.1. A proposed subsection (P-14.7) can be found on the Webboard:

http//www.webboard.rsc.org/IUPACVIII

For inorganic compounds, the revised Red Book recommends that the name be based on the order of citation of components in the formula, which is based first on the increasing number of each component and then alphabetically.

Although the 'inorganic' method may work for inorganic compounds, there can be problems when applied to organic compounds. The proposed subsection P-14.7 orders the components according to the hierarchy used in organic nomenclature as given in subsection P-41 of the new Blue Book. This method is very similar to the 'compd. with' method used by CAS. Hierarchical arrangement permits similar names for compounds differing only in the ratio of components.

It was noted that the method used in organic recommendations involving the use of parenthetical element symbols connected by a long dash to indicate a coordinate bond between the named elements should be contrasted with the method of coordination compounds; the latter seemed much more rational and easier to apply.

It was recommended that Meisenheimer complexes be removed from the proposed subsection P-14.7.

It was agreed that further consideration of this subject be carried out by a small group consisting of Dr K-H. Hellwich, Dr A. Yerin, Dr T. Damhus, and Dr W. Powell.

8.4 Preferred structure-based names for macromolecules

As soon as the final draft of the new Blue Book is finished, it will be necessary to evaluate its consequences for macromolecular nomenclature with a view to preferred structure-based names for macromolecules.

8.5 Boron nomenclature

Correspondence with Dr John Kennedy has indicated that he does not wish to lead a project on boron nomenclature. It was suggested to send a representative to the next IUPAC Boron Conference to try to find interest.

8.6 Other future projects

8.6.1 A second edition of the book "Principles and Practices of Chemical Nomenclature, A Guide to IUPAC Recommendations" published in 1998, authored by G. J. Leigh, H. A. Favre, and W. V. Metanomski.

[Secretary's note: Subsequent to the meeting, it was learned that according to the Secretariat's records, Blackwell has sold 1369

copies and the Secretariat has sold 116 for a total of 1485 copies. The list price is USD 30. There are 16 copies left in stock. About 20 copies have been given away over the years at conferences, etc.]

Prof G. J. Leigh is willing to organize such a project. Planning should take a year with actual work starting in 2006. Dr Hellwich volunteered to be involved. Suggestions as to content should be sent to Prof Leigh.

Content should include an emphasis on decoding names as well as coding them. Perhaps a list of abandoned trivial or common names and their systematic equivalents should be included. A historical introduction might be included.

8.6.2 Stereochemical nomenclature.

Chapter 9 in the new Blue Book describes, in detail, the use of descriptors in names. Description of configuration in coordination complexes with higher coordination numbers has been studied (see minute 7.5). Perhaps it is time for a full discussion of the principles of stereochemical nomenclature for both organic and coordination structures in a separate book.

Dr K.-H. Hellwich has proposed a project on conformation stereochemistry, but so far there has been no interest expressed.

The need to revisit stereochemical terminology should be examined.

8.6.3 Ambiguity in Names.

It was noted that there was a meeting at 4:00 p.m. today (August 14) in Hall 10 in the Beijing International Convention Center to discuss ambiguous terminology hindering trade. Dr K.-H. Hellwich attended. The meeting dealt with analytical terminology, in particular classification of traces of pollutants, i.e., purity of products. Similar problems may well occur with improper or ambiguous chemical names (see also minute 8.6.4)

8.6.4 Problems of those dealing with chemical names who know nothing about chemistry or nomenclature. Dr David Barden noted that Aldrich was used as an "authority" on nomenclature by at least some laboratories.

9.0 Committee Membership

9.1 Election of Titular Members has been completed. Dr G. P. Moss will continue as a Titular Member and assume the office of President. Dr A. D. McNaught will continue as a Titular Member and assume the position of Past-President. Dr W. H. Powell was elected for a further two-year term as a Titular member and Secretary. Drs Steve Heller and K.-H. Hellwich were elected as Titular Members for four year terms.

The complete list of Titular Members is thus as follows:

Dr Gerry Moss (President)
Dr Warren Powell (Secretary)
Dr Alan McNaught (Past President)
Dr Ture Damhus
Prof Richard Hartshorn
Dr Steve Heller

Dr Karl-Heinz Hellwich
Dr Jaroslav Kahovec
Prof Jozsef Nyitrai
Dr Andrey Yerin

9.1 Associate Members 2006-2007. The following was approved by the Division Committee in Beijing.

Mr Jonathan Brecher and Prof. G. J. Leigh will continue as Associate Members. Prof R. G. Jones, Dr J. Wilson, Dr A. T. Hutton, and Prof. F Cozzi were nominated as Associate Members and will be contacted concerning their willingness to accept this position. Assuming that the above four will accept their positions, the complete list of Associate Members will be as follows:

Mr Jonathan Brecher
Prof Franco Cozzi
Dr Alan T. Hutton
Prof Richard G. Jones
Prof. G. Jeffery Leigh
Dr Jeff Wilson

9.2 National Representatives 2006-2007. The current number of National Representatives is 9; we are allowed 10 for this biennium according to the special modification of the Division Rules (see Appendix V) approved for the Budapest meeting (see minute 20.1 in the Budapest meeting). Three current National representatives cannot be reappointed as they have reached their maximum years of service. The National representative from Argentina, Prof Rita Hoyos de Rossi, cannot be reappointed because Argentina has not paid its dues. Five National Adhering Organizations have nominated representatives. Hence, we have the following new National Representatives:

Prof Ivan Dukov (Bulgaria)
Prof S S Krishnamurthy (India)
Prof Youngkyo Do (Korea)
Dr Farzana Ansari (Pakistan)
Prof Martin Putala (Slovakia)

The list of reappointed National Representatives for 2005-2007 is as follows.

Prof Len Lindoy (Australia)
Dr Martin Ragnar (Sweden)
Prof Jan Reedijk (Netherlands)
Dr Paolo Righi (Italy)

[Secretary's note: Subsequent to the meeting it was learned that Argentina has paid its dues and therefore Prof Rita Hoyos de Rossi will be the National Representative from Argentina for 2005-2007]

9.3 Vice-President: procedure for election

It was agreed that the Division Committee should always retain three officers, President, Secretary, and Past President OR President, Secretary, and Vice-President.

Since we have the office of Past-President this year, an election of a Vice-President is not urgent and should be further considered at next year's meeting

9.4 Advisory Subcommittee 2006-2007. The current list of members of the Division VIII Advisory Subcommittee is given in Appendix IV. The following were nominated as new members. They will be contacted to be sure that they are interested in joining the Advisory Subcommittee.

Mr Thomas E. Sloan
Dr Robert Temme
Dr Kirill Degtyarenko
Dr Harry Gottlieb
Dr Elisabeth Weber

9.5 Election procedure

Because the procedure used for the Division VIII elections this year had been questioned, it was felt necessary that it be reviewed. The procedure for Division Elections is included as items 4-6 of the Division Rules of the Chemical Nomenclature and Structure Representation Division given in Appendix V.

Dr G. J. Leigh explained his objections to the procedure used for the 2005 elections and Dr G. P. Moss, who was the Chairman of the Nominating Committee for the 2005 elections, detailed the procedure that was used.

It was noted that there were necessary differences for Division VIII Committee elections from other Divisions, mainly which in addition to geographical constraints, the Division VIII Committee must possess acceptable knowledge of the whole range of nomenclature and cognate disciplines.

It was agreed to have a full discussion about the nominating procedure at the Division VIII meeting next year. The following suggestions were offered.

- Be more active in encouraging applications for the "young observers" program.
- Have data on the members whose terms are expiring available before the meeting in Prague.
- Provide more candidates for consideration.

10.0 Publicity

A publicity plan to be implemented when the new Red and Blue Books become available as noted in the Budapest minutes was still to be prepared. Publicity for the IUPAC colour books by RSC will no doubt be no more than that provided for other books published by RSC. Dr A. McNaught will try to generate a plan for publicity. Previous minutes contain lists of suggestions for methods of publicizing the work of Division VIII.

ACS Career Workshops had been successfully run in collaboration with other IUPAC Divisions but don't seem appropriate for Division VIII.

Other suggestions for publicity included:

(1) Build ways to highlight nomenclature matters in the new IUPAC website.

(2) Press releases about new colour books or new editions of nomenclature manuals.

(3) New book announcements in chemistry journals.

(4) Book reviews

(5) Publications on nomenclature problems and pitfalls.

(6) Letters and/or notes on nomenclature matters in journals.

11.0 Article for Chemistry International

Dr F. Meyers has requested a one page report on what Division VIII accomplished here in Beijing for publication in *Chemistry International* this fall.

12.0 Report from the Committee on Printed and Electronic Publications (Dr Steve Heller)

The IUPAC website is moving from Research Triangle Park (RTP) to the Fachinformationszentrum (FIZ) Berlin which is donating two servers to IUPAC. The move will occur in a three-step migration and duplicate sites will coexist for a while before the move is complete. The purpose of developing a new IUPAC website is to incorporate the Division VIII Webboard (now located on the RSC website) and the IUPAC and IUBMB Nomenclature Web Site (now located at Queen Mary College of the University of London and managed by Dr G. Moss). The work is being done under contract by a group in Prague. The Prague group has converted the IUPAC website to XML. Development of the IUPAC website is a major objective of CPEP.

13.0 IUPAC and IUBMB Nomenclature Web Site (Queen Mary, University of London)(Dr Gerry Moss)

13.1. Access statistics. The statistics on the use of the website are given in Appendix VI.

13.2. There have been problems with the old software used for the RSC website during the past year which affected the Division VIII webboard. New software has been installed.

13.3 Relationship with the IUPAC web site, and plans for the future.

The new IUPAC website must be developed before the IUPAC and IUBMB Nomenclature Web Site at Queen Mary can be incorporated. Dr Moss wants to be able to develop statistics from the IUPAC website just as he does now from the IUPAC/IUBMB website.

The mirror sites for the IUPAC/IUBMB website are not necessarily kept up-to-date.

14.0 Translations

Dr K.-H. Hellwich noted that *Angewandte Chemie* has had a policy to translate IUPAC Recommendations into German, but this has turned out to be a large task. A group of translators is needed to do this. A list of German translations of IUPAC recommendations is given in Appendix VII. Translations are quite valuable as many corrections and necessary modifications to the official IUPAC English publication may emerge. These corrections can be made to the online version but a printed correction or corrigenda may be necessary as well. This has already happened with the 1993 Guide to Nomenclature of Organic Compounds and with Natural Products (revised Section F of the 1979 Organic Recommendations); in both cases printed corrections have been published. And it is happening with both publications on fullerene nomenclature.

Project groups need to be very diligent in proofing their publications to minimize corrections and editorial modifications.

The Division must alert National Adhering Organizations (NAO's) about the publication of nomenclature recommendations and ask if translations are likely. NAO's should be encouraged to translate nomenclature recommendations. The difference between translations and interpretations must be recognized. Translations need approval by the appropriate NAO.

It was suggested that a publication for *Chem. Int.* about translations could be useful.

15.0 Cross representation from the Division VIII Committee to other IUPAC Committees

15.1 Committee on Chemistry Education (CCE). Dr T. Damhus will attend the meeting of CCE here in Beijing this year. Prof R. Hartshorn will be Division VIII's representative starting next year.

15.2 Committee on Printed and Electronic Publications (CPEP). As a member of CPEP, Dr S. Heller will serve as Division VIII's representative

15.3 Committee on Chemistry and Industry (COCI). At present Division VIII does not have a representative on this committee. Dr A. McNaught will attend this committee's meeting this year here in Beijing and will attend its meeting next year if no one else is willing.

15.4 PAC Editorial Board. Dr A. McNaught will attend the meeting of this committee this year here in Beijing and will carry on to succeeding years if appropriate.

15.5 Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS). Dr A. McNaught will replace Dr W. V. Metanomski as a Titular Member. Prof J. Nyitrai will be Division VIII's representative. Prof J Kahovec currently represents Division IV (Macromolecular Chemistry). Dr T. Damhus remains as a Titular Member. There was discussion concerning the double Titular membership of T Damhus in Division VIII and ICTNS.

16.0 Next meeting

Dr. J. Kahovec invited the Division VIII Committee to meet next year (2006) at the Institute of Macromolecular Chemistry in Prague. The proposed schedule was to have meetings of Project Task Groups on September 4-5, 2006 and the meeting of the Division Committee on September 6-7, 2006. These dates must still be confirmed by Dr Kahovec.

Respectfully Submitted: Warren H. Powell (Secretary) 11/25/05

Accepted: Alan D. NcNaught (President) 11/30/05

APPENDIX II

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

Minutes of the Annual NC-IUBMB and JCBN Meeting Bonn, Germany, May 13-14, 2006

Attendees:

NC-IUBMB and JCBN

Richard Cammack (London, UK)
Keith Tipton (Dublin, Ireland)
Hans Vliegenthart (Utrecht, The Netherlands)

NC-IUBMB

Dietmar Schomburg, Chairman (Cologne, Germany)
Helen Berman (Piscataway, NJ, USA)‡
Minoru Kanehisa (Kyoto, Japan)

JCBN

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

Others

Rolf Apweiler (Hinxton, UK)	Associate Member of NC-IUBMB
Hal Dixon (Cambridge, UK)	Associate Member of NC-IUBMB
Derek Horton (Washington, DC, USA)	Associate Member of NC-IUBMB
Toni Kazic (Columbia, MO, USA)	Associate Member of NC-IUBMB
Alan McNaught (Cambridge, UK)	Associate Member of JCBN
Donald Nicholson (Leeds, UK)	Associate Member of NC-IUBMB
Kristian Axelsen (Copenhagen, Denmark)	Observer
Ture Damhus (Copenhagen, Denmark)	Observer (IUPAC: ICTNS, Division VIII Committee)
Karl-Heinz Hellwich (Frankfurt, Germany)	Observer
Sabine Kuhn (Columbus, OH, USA)	Observer
Ida Schomburg (Cologne, Germany)	Observer

‡Attended meeting on May 13 only

1. Welcome and Apologies

Apologies were received from Athel Cornish-Bowden, Alan Chester, Charles Cantor and Arnost Kotyk. Schomburg welcomed the Committees to the meeting and apologized for the change of venue from Cologne to Bonn.

2. Approval of Agenda

The agenda was approved without modification.

3. Minutes of the Columbia Meeting, May 2005

These were approved as a record of the proceedings of the Columbia meeting.

4. Matters Arising

There were no matters arising other than those listed in the current agenda.

5. Reports

5.1 Chairman's Report (Schomburg)

Schomburg reported that he became Chairman in January of this year and that there were a number of things that he wanted to improve. Our responsibilities can be divided into two broad areas: general biochemical nomenclature, which comprises proteins, nucleic acids, carbohydrates and other molecules of biological interest (including steroids/terpenoids and alkaloids) and the classification of enzymes, comprising new classes/subclasses/sub-subclasses/entries and the correcting/updating of existing enzyme entries.

Schomburg said that we have been active in some of these areas, but not all. Enzyme classification has always been the main activity of the Committees but we should also cover the other areas of responsibility. He reported that there have been dramatic changes in recent years regarding the use of the enzyme-classification system, as illustrated by the following results of Google searches.

Search terms	**Hits (Pages)**
'EC number' alone	2,300,000
'EC number' AND “Pathway”	755,000
'EC number' AND 'genome'	987,000
'EC number' AND 'disease'	693,000
'EC number' AND 'kinetics'	9,000

The number of hits when EC number is combined with the terms 'pathway', 'genome' and 'disease' provides an insight into the way that the importance of EC numbers has increased over recent years. The Environmental Protection Agency (EPA) also is considering the use of EC numbers as one of the prime methods of identification. Unique identifiers are essential to find relevant information in the literature, property and pathway databases. EC numbers are now used for a large variety of different tasks, including genome annotation, pathway reconstruction, systems biology etc.

Schomburg stated that there are a number of problems, either real or perceived, with both the enzyme data and the procedure for enzyme classification. Inconsistencies in the enzyme data provided at different locations are a major problem. He said that the decision was taken in 2001 that IntEnz would become the master database and that all data would be entered directly into this database. However, because of problems with data input into IntEnz and output in a form that was satisfactory for Moss to incorporate into the Enzyme List at , IntEnz is no longer being used by the Dublin group. The current situation is that changes are copied manually from Moss' website into IntEnz. As a consequence of the problems with IntEnz, the Dublin group have developed a MySQL database ( ) and data are now output from that database for direct inclusion on Moss' website. This should solve the problem of inconsistent datasets. Schomburg reported that, up until now, it has been difficult for information providers to access the enzyme data, which they

have had to manually copy or parse from the information on Moss' website. Reported problems of inadequate feedback to submitters and a general feeling that the "Enzyme Commission is slow" need to be addressed.

Schomburg reported that he has had discussions with the Dublin group and that agreements have been reached. All changes to enzyme data are now made in a MySQL database, which is available for download by interested parties. Replication of the database between Dublin and Cologne groups has been set up and this works well. He said that tracking of changes is not yet included in the downloadable version and this should be addressed (**Action:** Dublin to include timestamps for all fields in which data have been modified; NOTE by Boyce: this has been implemented). Forms for the submission of data on new enzymes and error/updates to existing entries have been set up in Dublin (and) but automatic feedback to submitters is not provided (feedback to individuals who submit data is by e-mail). Schomburg would like a more transparent system whereby submitters can see the status of their submission online, although that need not replace the “more personal touch” of direct e-mail communication.

Schomburg said that we should identify new enzymic activities in a more systematic way, e.g. using text-mining tools, as used by the BRENDA team, or Kanehisa’s research methods associated with KEGG. We also need to identify more experts to help with specific groups of enzymes. He said that the data must be kept in an updatable repository and that the inclusion of the dates of all changes must be enforced. The name of the person making the changes should also be included and all changes should be archived, along with the reason that changes were made. He said that the archive must be stored at several locations and, in accordance with the 2001 decision, he would like the EBI to guarantee its long-term availability.

It was agreed to replace 'Common name' with the term 'Accepted name' as it was felt that this term was stronger and might make it easier for editors to enforce its usage. Ture Damhus indicated that IUPAC Division VIII have approved the use of just three terms: 'Not acceptable', 'Preferred' and 'Acceptable' and said that it was unfortunate that closely related bodies had different naming preferences. (**Action:** Boyce to replace 'Common name', and 'Recommended name' for enzymes in EC 3.4, with 'Accepted name').

Schomburg reported that e.g. the UniProt, KEGG and BRENDA teams are frequently finding new enzyme activities and said that we should formalize cooperation with these. Additional people are needed to help with these activities and we should get help from more external experts. He has applied to the Beilstein Foundation on behalf of the Committees, for a grant in support of enzyme nomenclature, some of which could be used to pay honoraria for such assistance. He also said that we need to increase awareness in the community that EC numbers are assigned only by the IUBMB. Kazic asked who would be responsible for quality control and Schomburg indicated that this will remain with the Committees. Dixon reported that, when he needed advice on a particular enzyme, he often wrote to the corresponding author of a key paper. He said that it might present a problem if some people were paid for their advice and others were not. Apweiler said that there was a need to enlarge the number of people devoted to the task and suggested that other groups that deal with enzymes, e.g. CAS, could advise/supervise implementation of a larger group classifying enzymes. He said that there is a need for a core of people who are responsible for day-to-day management, with the Committees being an advisory board to those who actually do the work.

Apweiler also reported that Mike Gribscov and Susan Taylor are communicating with UniProt regarding the classification of protein kinases (NOTE by Boyce: major reclassification and expansion of the list of protein kinases was completed in 2005 after a period of public review and these enzymes have been incorporated into the official Enzyme List. At the 2005 meeting, Berman had agreed to ask Susan Taylor for her input on these enzymes when they were at the public-review stage, but no feedback was received).

Additional proposals by Schomburg were to extend our activities to include other protein classes in collaboration with experts in those areas, e.g. TRANSFAC for transcription-factor data and IUPHAR's work on transport proteins. He said that we should find groups that maintain databases on particular areas of nomenclature. We could then study the nomenclature systems they use and, if appropriate, we could recommend their usage. Apweiler reported that UniProt have drafted guidelines on how to name proteins as there are no existing standards. It was agreed that the UniProt document should be distributed with the Minutes and we will determine if this is the sort of activity that we should consider (**Action:** Boyce to distribute UniProt document with the Minutes).

In relation to having additional experts involved in enzyme classification and nomenclature, Schomburg said that he would like to enlist experts that could be responsible for different classes of enzymes and to name them as experts on the enzyme website. McNaught agreed that this might be a good idea. Tipton pointed out that, in this context, “classes” need not necessarily correspond to EC classes, but rather to substrate groups. Apweiler suggested that editorial boards be asked for lists of people working in particular areas and that we pay these experts on an enzyme-by-enzyme basis. He said that the naming of experts was a good idea but financial remuneration was also important if we wished to receive responses in a timely fashion. It was agreed that those offering significant advice on specific enzymes should be acknowledged on the website and that the names of those making major contributions to the nomenclature and classification should be prominently displayed (**Action:** Moss and Schomburg, website). Cammack reported that he had had discussions with Patsy Babbitt [from the University of California at San Francisco (UCSF)] and she was interested in becoming involved in enzyme classification.

Another initiative that Schomburg would like to implement is to extend our activities in the area of small molecules in cooperation with ChEBI. Currently, ChEBI has fields for synonyms, one for IUPAC names and one for the commonly used name. McNaught reported that none of these names are considered to be a preferred name. It was suggested that the primary term for those molecules that occur most frequently in the Enzyme List should be identified. It was agreed that an application should be made for IUPAC funding for a project on small-molecule nomenclature. The group involved will be Marcus Ennis (approved as an associate member of the NC-IUBMB), Gerry Moss, Kirill Degtyarenko, Hal Dixon, Susumo Goto, Toni Kazic, Jaroslav Kahovec ( ) and someone from the BRENDA team (**Action:** Cammack to coordinate application to IUPAC).

In relation to the enzyme data, Berman wanted to know explicitly what version of the Enzyme List is the authentic one and where it is located. She said that there must be only one master copy of the Enzyme List and that only one group should have write-access to that. She said that everyone should sign up to say that they will not corrupt the

data in the master database and agree to update their database so that the data remain consistent.

Apweiler said that he had received a guarantee from the Committees in 2001 that the master copy of the data would reside at the EBI until such times as they could no longer afford to maintain it. He said that they had developed the IntEnz database for this purpose at considerable expense. He said that this remit had not been revoked and that he would consider it a breach of contract if it was revoked. Boyce indicated that this was not an accurate account of the agreement that was reached as it was agreed that this decision could be reviewed by the Committees after cessation of the BioBabel grant (end of 2004) (NOTE: Minute 8.1 of the 2001 Minutes, copied below). She also reported that there were serious problems with the IntEnz database that had not been remedied by the end of the grant and this was the reason that the Dublin group had had to develop their own database. These problems included unavailability of the curatorial tools for variable periods of time, no provision of html output for Gerry Moss in the form that he uses at the qmul website, as agreed at the 2001 meeting, and most serious, data entered into the database were often lost (either all of the data from a particular field or, more difficult to spot, partial loss of data from fields). These problems resulted in an increased workload, which adversely affected new enzyme classification, and made it very difficult to keep track of data.

It was agreed that we need one master copy of the data. It was also agreed that the database archive will be stored at the EBI. Schomburg said that this does not imply that the EBI can make any changes to the data in the database. However, they would be responsible for guaranteeing its long-term availability. (**Action:** Schomburg to draft contract to this effect). The database should be available for download by anyone for both internal use and redistribution. Apweiler suggested that this be made available under the Creative Commons Attribution – Noderivs Licensing Scheme, which means that the data would be freely available but that those who download it cannot change the data and they must attribute the data to the IUBMB. Changes to the data remain the responsibility of the Committees. Licensees must also agree to keep the data up to date. It was also suggested that we could get data repositories in Japan/USA. These would have to be places with stable computers, daily back-ups etc.

5.2 Treasurer's Report (Cammack)

Cammack noted that we need to keep track of expenditure and to keep within budget, especially with respect to the IUBMB budget. He reported that the budget from the IUBMB is $15,000 in total for the period 2005-2007. He asked that those attending the annual meeting next year inform him of their intention to travel before they make their bookings. In order to claim expenses for the 2006 meeting, members funded by IUBMB should contact Cammack. He hoped that the funding obtained could also be used to contribute to expenses incurred attending external meetings, such as the meeting that took place on May 12 of those actively involved in enzyme classification. He also pointed out that the funding has to be used to contribute to the meeting costs incurred by the host. Funding by IUPAC operates under a different system whereby participants receive a per-diem payment ($170 for attendance at the meeting in Germany) plus travel costs. He reported that the IUBMB are considering moving to a similar per-diem system. Cammack reported that IUPAC has considerable funds available for projects, which are awarded on a competitive basis. If a project is approved, then the funds awarded can be used to pay for meetings of participants to discuss the project.

6. Name of the Committees (Schomburg)

As the Committees comprise two different bodies and three different types of membership (membership of JCBN, of NC-IUBMB or of both the NC-IUBMB and JCBN), Schomburg suggested that we decide on an umbrella name to refer to the Committees. His suggestions were "Joint Committee on Biochemical Nomenclature" (JCBN) or "Joint Committee on Biochemical Nomenclature and Enzyme Commission" (JCBN-EC). Dixon said that he was not in favour of these suggestions as they (1) had the same initials as the JCBN and (2) were rather long names. He suggested "International Biochemical Nomenclature Committee" as an alternative. Berman said that there was an advantage to having a name with the same initials as the JCBN in that there is some sort of branding. It was agreed to use the name 'Joint Committees on Biochemical Nomenclature' as an umbrella term when referring to the two committees. Schomburg reported that he has reserved the website addresses and and that they currently provide a link to Gerry Moss' web pages. Dixon thought that IUPAC and IUBMB would not be affected by us having an umbrella name, but requested that they be informed of this decision (**Action:** Schomburg to inform IUBMB and IUPAC of this decision).

7. Enzyme Nomenclature and Classification

7.1. Necessities of enzyme classification in the post-genomic/systems biology era (Schomburg)

This was not discussed as a separate item as it had been covered in Item 5.1.

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

During the past year, 162 new enzymes have been added to the Enzyme List. In addition, 66 entries have been modified extensively, 38 enzymes have been deleted/transferred and numerous other enzymes have had minor changes made to them.

In order to make the activities of the Committees in relation to enzyme classification and nomenclature more transparent and to improve the service provided, a number of initiatives are being implemented. A Frequently Asked Questions document has been drafted, which will provide information on such things as the procedure involved in classifying an enzyme and the timeframe involved.

To address the problem that enzyme classification is considered a very slow process, a number of initiatives are being implemented to reduce the time between submission of data on a new enzyme and its inclusion in the official Enzyme List. Our previous practice was to have batches of enzymes that underwent public-review for a period of two months. Significant improvement in this time frame (currently four months for an enzyme received just after a batch has been published) will be achieved by changing from the batch system to the review of individual enzyme entries, which can be added to the public-review site as soon as they are ready. It was agreed at the meeting that the time for public review would be reduced from two months to four weeks, which will also reduce the time involved. The date on which an EC number will be made official will be appended to each new enzyme so members are asked to check the enzymes undergoing public review (available at

or

) regularly. We will also be more active in informing interested parties when new material is available.

Data can be output from the database in the form used by Moss on his website, which should prevent inconsistencies occurring between the two data-sets.

Tipton pointed out that the transfer of enzymes from one EC number to another is not always the result of errors on our part – new information on many enzymes results in their transfer to more appropriate EC numbers.

7.3 **Request for suggestions for appointment of members with expertise in the areas of nucleic-acid enzymes and peptidases (Tipton)**
Tipton pointed out that we no longer need to look for an expert in the area of peptidases as Ida Schomburg has done considerable work in updating the peptidase entries for the Enzyme List. He also reported that Alan Barrett had written to him suggesting that, since the basis for peptidase classification differs from that used for other enzyme classes, we should list only three or four peptidases, based on specificity, and refer users to MEROPS to find more detailed information. Tipton consulted other peptidase experts about this suggestion (including Tony Turner and Karl Bauer) and they were strongly against this suggestion.

Ida Schomburg gave a brief report on the work she has carried out on drafting peptidase entries. She checked all entries in MEROPS that do not have EC numbers and searched for literature that provided the details required for characterization. Of the 122 peptidases that had some publications, she considered 60 of these to be sufficiently characterized to warrant classification. She had sent initial drafts to Boyce and Tipton for comment and, after some further work on the “Accepted names”, she will provide revised material from which Boyce will produce the entries for the Enzyme List. Links will be provided to the relevant MEROPS entries but it was agreed that the MEROPS recommended names will not necessarily be used as our Accepted names, although they would be included in the lists of synonyms (**Action:** Ida Schomburg to revise data and Boyce to draft entries).

An expert on nucleic-acid-related enzymes is still needed and Tipton asked for suggestions of people who could be approached. Cammack suggested that David Lilly of St. Andrew's be contacted and Tipton agreed to do this (**Action:** Tipton to contact David Lilly). Kazic said that she will also try to contact some possible experts (**Action:** Kazic).

7.4 **During the past year, we received a number of complaints from Prof. Jack Kyte, University of California, about changing the common names of enzymes. Having replied saying that the only time we change a common name is if it is (a) not a commonly used name for the enzyme or (2) incorrect or misleading, we agreed to raise this issue at the Nomenclature meeting.**
It was agreed that we should change accepted names only for very important reasons but will continue to change names if they are either misleading or incorrect. The example that Prof. Kyte cited was originally called "dihydrolipoamide *S*-acetyltransferase" (EC 2.3.1.12) but that name has since

been changed to "dihydrolipoyllysine-residue acetyltransferase". Dixon reported that Richard Perham, and expert in the field, had been consulted on all of the names shown for the oxo-acid dehydrogenase complexes ( ). The reason for the change of name was that it was now known that the natural substrate of the enzyme is the dihydrolipoyl lysine-residue, and not dihydrolipoamide. (**Action:** Boyce to include the reason for name changes in the FAQ and Tipton will inform Prof. Kyte of the decision reached).

7.5 Correspondence with Dr. Ron Caspi of MetaCyc who feels that each individual reaction should be given a separate EC number

Ron Caspi believes that we should not classify enzymes but rather that we should classify the reactions, e.g., each reaction catalysed by alcohol dehydrogenase (EC 1.1.1.1) should have a separate EC number, as should consecutive reactions. Axelsen said that, from a bioinformatics point of view, it would be preferable to have one reaction per EC number. Kanehisa said that the Committees make an experimentally verified list of enzymes, but said that the species and gene upon which the entry is based should be made clear in enzyme entries. He said that the number of reactions in known pathways with no EC numbers is large. He also pointed out that they have a reactions database and that, while reaction specificity is straightforward, substrate specificity is a problem. It was decided that there was nothing we can do as our function is to classify enzymes and not reactions.

7.6 Dr. Peter Karp's proposal for differentiating between different types of incomplete EC numbers (those where it is assumed that an enzyme must exist but there is insufficient characterization to warrant an EC number and those where an EC number could be issued based on the evidence available) (Schomburg)

Partial EC numbers are used for two different purposes: (1) to indicate those enzymes that do not have a full EC number but are sufficiently characterized to warrant an EC number and (2) those that are not sufficiently characterized, but that the author assumes would belong in a particular sub-subclass. A dash is often used to represent both of these cases (e.g. 1.1.1.-). Karp (in his paper at) has recommended the use of 'n' for case (1) (e.g. 1.1.1.n) and the use of a question mark for case (2) (e.g. 1.1.1.?). This paper had been sent for comment to Boyce and Tipton before publication and they had expressed support for these proposals. Kazic suggested that we should discuss this with PubMed before embarking on any such recommendation. Axelsen said that the use of the question mark may not be a good idea. In response, Schomburg said that Amos Bairoch also approved of Karp's symbolism. Apweiler said that he supported the proposals in principle but that removal of the ambiguity associated with the dash depended on users using the symbols 'n' and '?' in the correct way. Schomburg, Axelsen, Apweiler and Kazic will look into the details. If they find no reasons to reject the proposal within the next four months, we will recommend it. Schomburg will also discuss the proposal with people from The EMBL Nucleotide Sequence Database, KEGG and UniProt. Tipton suggested that we publicize the proposal on the web and ask for feedback. This was agreed. (**Action:** Schomburg,

Axelsen, Apweiler and Kazic to determine if there are any reasons not to implement this system; Schomburg to discuss the proposal with people from The EMBL Nucleotide Sequence Database, KEGG and UniProt, and Moss to include a note on the proposal on his website along with a request for feedback).

7.7 Update on amine oxidases (Tipton)

Tipton reported that he had a complete draft that he sent to several concerned people but he is still waiting for a reply from a plant/fungus expert before he circulates it to the Committees.

7.8 Isomerases that are energases (Tipton)

The issue of separating isomerases on the basis of whether or not they use NTP was settled with the decision being made not to differentiate on this basis. Tipton reported that he is in the process of preparing the list and will send it to Boyce to include in the enzyme database. (**Action:** Tipton to send Boyce revised list of isomerases).

7.9 Ribonuclease (Tipton)

Tipton reported that, in 2005, the International RNase Congress yet again asked that EC 3.1.27.5 (pancreatic ribonuclease) be reclassified since it is not a hydrolase. They would like it to be a transferase (it was between 1961 and 1972, as EC 2.7.7.16) but they would be content for it to be a lyase. It was agreed to reclassify it as a lyase (**Action:** Boyce to reclassify this enzyme).

7.10 Standards for reporting enzyme data (Tipton)

Tipton reiterated that standards for the reporting of enzyme data are being drafted by the STRENDA committee. The Committees have already approved the first STRENDA document (Level 1, List A - on required data for e.g. Materials & Methods section of publications). The second document (Level 1, List B: Reporting Enzyme Data*)* is at the preliminary draft stage and is available for comment at . The final document has the title "Level 2: Organism-related Definitions of Experimental Conditions" and is at the stage where they are consulting experts.

Apweiler reported that there will be a Nature Biotechnology focus issue on standards for reporting life-science data. A lot of data will come from the proteomics standardization group. The editor encouraged Apweiler to submit the STRENDA documents for inclusion in this issue. It was agreed that we recommend the STRENDA documents.

7.11 Publicity and information

Moss provided details of the usage of his website, broken down into the various types of data that were accessed (see Appendix I). Dixon also mentioned that a much improved version of the Gold book is available online at

.

8. Items for Discussion

8.1 Report on meeting with IUBMB Executive on the work of the Nomenclature Committees and future funding (Cammack or Schomburg)

Cammack reported that he gave a presentation on the activities of the Committees to the IUBMB Congress on July 1 2005. There is a requirement in the statutes of the IUBMB to support nomenclature activities. Cammack reported that one of the successes of the Committees' activities has been the nomenclature website run by Moss. He also reported that summaries of nomenclature recommendations can be published in IUBMB Life on an annual or biannual basis.

Schomburg reported that, in general, the IUBMB was very supportive of our work but they had criticized the speed and transparency involved in the process.

8.2 Report on meeting with FIFRA Scientific Advisory Panel on enzymes for the US Environmental Protection Agency (Cammack)

Cammack reported that he had attended a meeting with the US Environmental Protection Agency (EPA) in May 2005. The EPA have to name compounds for inclusion in their inventory. Until recently, they did not include enzymes. For each enzyme, they have a description based on function, sequence, source and how the enzyme has been processed. Many of these enzymes do not have EC numbers as they are often not purified (e.g. could be found in pig pancreatic extract rather than be a purified enzyme).

Questions relating to enzyme function were asked at the meeting and it was felt that the function should carry the highest weight of the four parameters above. Detailed minutes of the meeting are available at . They wanted to know if an enzyme was produced by engineering or extraction from an unknown source, could the enzyme be given an EC number. Cammack had stated that it should be possible to create an EC number for an enzyme so long as its specificity had been explored sufficiently. It was agreed that there would not be a problem providing EC numbers for engineered enzymes. According to EPA rules, an EC number would have to be provided within 90 days of submission. Tipton stated that, with the initiatives taken to reduce the time between submission of an enzyme and assignment of an official EC number, this should not be a problem provided that sufficient data were provided. Cammack has raised the issue of remuneration for this work with the EPA but no agreements have been reached. Sabine Kuhn raised her concern that the EPA are strongly opposed to data being changed, so, for example, if it turned out that an EC number had to be changed, the EPA could object to the change being made. Discussions are ongoing between Cammack and the EPA (**Action:** Cammack to continue discussions with the EPA).

8.3 Update on Nicholson minimaps and animaps (Nicholson)

Nicholson reported that the 22nd edition of the large metabolic map produced by Sigma-Aldrich is now available
(
). He thanked the Committees for their continued support of his activities and reiterated that the copyright for his charts, minimaps and animaps lies with the IUBMB. He said that the IUBMB had obtained considerable money over the past five years from Sigma-Aldrich as a result of his metabolic charts. Some of this money is used to sponsor attendance at conferences by researchers from developing countries who otherwise would

not have the money to attend international meetings. NIcholson reported that the 'inborn-errors of metabolism' map is being extensively revised at present. He is currently concentrating on the provision of animated maps, as he feels that these will engage students more than static maps and will bring the chemistry to life for them. Web versions of four animaps have been prepared by Andrew McDonald in Dublin and are available at). Nicholson is currently working on one to illustrate the mitochondrial respiratory chain. Nicholson gave a demonstration of the reactions that take place in the pyruvate-dehydrogenase complex.

8.4 Should we standardize on a single method for indicating locants in chemical names? (Dixon and McNaught)

Locants are used to indicate the position of a functional group within a molecule. In the Enzyme List, we use two methods to indicate locants: for amino acids, we use a superscript whereas for other compounds, largely carbohydrates, we add a number and hyphen before the atom to which the substituent is attached, e.g. N^5-acetyllysine but 4-*O*-methyl-D-xylitol. Dixon said that, If we wanted to move to a single system, this would be an excellent time to do so as the recommendation could be included in the new edition of the Blue Book, which will be published in 2007. This change would apply particularly to amino acids and sugars, since these are known by their trivial names. Horton pointed out that there are far more substituted carbohydrates than substituted amino-acids so it would be better to change the system for amino acids. Dixon said that if a decision is made to change the current system, then JCBN approval would be required. McNaught said that such a change could be processed as an erratum, which would be relatively straightforward. McNaught said that we should only consider the case of "N" followed by a numerical locant (as a superscript). It was agreed that we will change the system for amino acids so that a single naming scheme is used for all locants (**Action:** Schomburg to notify IUPAC and IUBMB of this change and Boyce to implement associated changes in the Enzyme LIst; McNaught to draft a corrections notice on the subject of locants for publication in Pure and Applied Chemistry. Once approved by the Comittees, this will need to go through the IUPAC review procedure before final approval).

8.5 Doubly substituted peptides. Moss asked that this item be raised after a request from Dr Hellwich of the Beilstein Institute

Dr. Hellwich attended the meeting so he described the problem that he had encountered. In the case of amino-acid or peptide sequences, an amino acid can be doubly substituted but there is no recommendation on how this should be indicated in print. He said that one author had inserted both substituents separated by a comma before the amino-acid symbol and that this could be with or without parentheses enclosing the substituents. Hellwich suggested that a recommendation on how to deal with this situation should be added to the Nomenclature and Symbolism for Amino Acids and Peptides document ( ) as a minor addition. Dixon expressed concern about the use of parentheses as these are used to express side-chain modifications. It was agreed that Moss, McNaught, Hellwich and Dixon will draft recommendations (**Action:** Moss, McNaught, Hellwich and Dixon to draft recommendations on how to indicate doubly substituted peptides).

8.6 Proposal for one- and three-letter codes for pyrrolysine (Apweiler)

Apweiler reported that pyrrolysine is the 22nd naturally occurring amino acid and that there have been a number of publications about this compound. However, there is a need for a clearly defined way of representing pyrrolysine in sequence databases so a one-letter and a three-letter code were needed. Apweiler recommended that we accept the suggestions of the NCBI to use the letter 'O' as the one-letter code and 'Pyl' for the three-letter code. Boyce pointed out that the three-letter abbreviation 'Pyl' is already used in the Enzyme List for EC 6.1.1.25, lysine-tRNA^{Pyl} ligase. This was agreed to. (**Action:** Boyce to draft a Newsletter item to this effect). Any such change should also be included in the amino-acid document.

8.7 Small molecules (Schomburg)
This was dealt with under Item 5 as part of the Chairman's report.

9. Update on Action Items from the Minutes of the 2005 Meeting

9.1 Membership procedure. Cammack said that we should have a term limit for the position of full member and Berman agreed to send him a document that she had on membership procedure (Minute 6.5: Action by Berman)
No action yet by Berman.

9.2 Cammack to relay to McNaught the terms of membership to the JCBN and McNaught to complete the necessary paperwork (Minute 6.5: Action by Cammack and McNaught)
This has been completed. Rules are different for members and associate members. The JCBN terms of reference were amended in 2002, resulting in a reduction in the number of IUPAC-funded members on the Committees (from four to two). The terms of reference are available at
. The IUBMB terms of reference for the NC-IUBMB (1999) are available at

.

9.3 Cammack to get suggestions for new Associate Members from the IUBMB. He also agreed to contact Richard Roberts of Nucleic Acids Research as part of an initiative to invite journal editors to become Associate Members (Minute 6.5: Action by Cammack).
Cammack suggested that Patsy Babbitt from UCSF, whose area of interest is how protein structures mediate protein function, be considered for associate membership of the Committees. (**Action:** Cammack to send further details).

9.4 Moss to approach Chemical Abstracts regarding nomination of a representative to the Committees as an Associate Member (Minute 6.5: Action by Moss).
This has been done. Margaret Holdemann from CAS will be made an associate member of NC-IUBMB with a start-date of 14 May 2006. Moss said that the issue of data exchange between the Committees and CAS is a separate issue that is under negotiation.

9.5 Cammack to issue invitation to Marcus Ennis to become an Associate Member. Also, Cammack to write a "Bitesize nomenclature" document on

the nomenclature of organic molecules of biological interest following discussions of this topic with Ennis (Minute 6.5: Action by Cammack).
Marcus Ennis has been invited to become an associate member of JCBN and his official term will begin on January 1 2007. It was noted that the tenure of an associate member is a maximum of ten years. No action has been taken on the nomenclature document.

9.6 Cammack to write to both Committees to have Don Nicholson appointed as an Associate Member of the NC-IUBMB and will provide an updated Membership List on the website (Open Forum: Action by Cammack).
Cammack reported that he had done this verbally at the meeting in Budapest.

9.7 Berman stated that she would like to provide Frank Allen of the Cambridge Crystallographic Data Centre (CCDC) with a business model to help them through their current financial difficulties and that would also allow the Committees access to the information in the CCDC's database (Minute 7.5: Action by Berman).
Berman has not taken action on this.

9.8 McNaught to instigate dialogue between Frank Allen and the Chairman of the RSC and to inform Allen of our willingness to provide letters of support, if requested (Minute 7.5: Action by McNaught).
McNaught reported that he has had many discussions with Frank Allen. He said that his offer of a letter of support was appreciated but was not required.

9.9 Kanehisa agreed to send Boyce a list of those enzymes that they found to be assigned different EC numbers using their automated method. (Minute 7.2: Action by Kanehisa).
Kanehisa said that he had not sent this list as he had been unhappy with the assignment of the fourth digit obtained using his software. He said that he would provide Boyce and Tipton with a copy of the software that they use for E-zyme.

9.10 Moss to ask Dixon to look into the incorporation of up-to-date nomenclature into the Cyclic Peptides document (Minute 7.5: Action by Moss).
This has not been updated yet.

9.11 Lipid MAPS. Cammack to ask Chester if he would be willing to undertake this project and to communicate with Lipid MAPS people (Minute 7.6: Action by Cammack).
No action taken. This item is not to be added to future agenda.

9.12 Schomburg to provide comments on new protein-kinase entries to Boyce, and Berman to ask Susan Taylor to provide feedback (Minute 8.1: Action by Schomburg and Berman).
The protein-kinase revisions have been incorporated into the Enzyme List. There was no feedback from Berman or Susan Taylor.

9.13 Tipton to circulate revised amine-oxidase entries for comment (Minute 8.3: Action by Tipton)
Tipton is awaiting feedback from one of the experts that he consulted before proceeding with this.

9.14 Moss to check the validity of the entry EC 5.99.1.1 (Minute 8.4: Action by Moss)
No action taken.

9.15 There is an apparent anomaly in the definitions of oxygenases regarding dioxygen. Sub-subclasses 1.13.11 and 1.14.12 should be based on whether one or two oxygens are incorporated into the substrate(s), regardless of whether the oxygen atoms come from the dioxygen or from water. The definitions of these sub-subclasses should be amended accordingly. (Minute 8.5: Action by Moss and Dixon)
The wording has been agreed upon but the website has not yet been updated.

9.16 We should provide a Frequently Asked Questions (FAQs) page in which we could outline what is required to classify an enzyme and the timescale that is normally involved between submission of a suggestion and inclusion of the enzyme in the Official Enzyme List (Minute 8.9: Action by Boyce, Moss, Tipton and Dixon)
A draft FAQ has been prepared by Boyce. Once revisions have been incorporated, Boyce will circulate it and would welcome comments/suggestions. (**Action:** Boyce to circulate FAQ document)

9.17 Indication of charge in reaction equations, particularly in relation to NAD/$NADH_2$ vs. NAD^+/NADH + H^+. Tipton reported that Goldberg was disappointed with our decision to revert to charged forms and agreed to contact Cornish-Bowden and Goldberg to see if they could estimate the number of users who favoured the uncharged version of reaction equations (Minute 8.8: Action by Tipton)
Tipton reported that Bob Alberty is now realizing that many people are against his recommendation and that, although we tried to implement it, responses from users of the Enzyme List caused us, after discussion by the Committees, to revert to the use of NAD^+/NADH + H^+ etc.

9.18 Horton to finalize his article on carbohydrates for consideration as one of the "Bitesize nomenclature" documents (Minute 8.10: Action by Horton).
Horton reported that he does not have a formal draft ready yet but he does have a general plan. The 92-page carbohydrate document addresses most problems that people encounter. He plans to draft a simplified version of the document for biochemists, which will address source-based names that have been superceded and will be approximately 20-pages long.

Horton said that he would agree to modify Section F
( ) as well as the cyclitol section
( ). Hellwich said that the carbohydrate document is the most highly regarded of the chemical-nomenclature documents and that there was no need for a completely revised version of the document. Moss agreed with Hellwich and said that there should also be a section on cyclic polysaccharides. Kanehisa indicated that monosaccharide codes are the most important from a database perspective. McNaught suggested that more advice should be provided on glycoside conjugates, as should an explanation of how to decide what the parent compound is. Dixon reported that the short form used for

describing oligosaccharides allows for the inclusion or exclusion of hyphens to indicate bonds and he asked that the hyphenated form be used as this would be helpful to users. Horton said that database people should be brought in to work on this and suggested the inclusion of Claus-W. von der Lieth. von der Lieth has a BBA publication and an in-press article in Glycobiology. Horton said that he hopes to have a rough draft of the 20-page document prepared well in advance of our 2007 meeting. Apweiler said that he would like von der Lieth invited to our next meeting as an expert and this was agreed (**Action:** Schomburg will contact von der Lieth and invite him to our next meeting).

9.19 Attempt to achieve consensus on a standardized format between the two groups proposing iconic symbolism for carbohydrate nomenclature. (a) Horton to send Boyce details of these systems for distribution with the Minutes (Minute 9.16: Action by Horton) and (b) Cammack said that he would like for us to provide links to both sets of iconic symbols from our website but without recommending them. He agreed to write to both groups and let them know what we plan to do (Minute 9.16: Action by Cammack)
Horton said that consensus between the two groups was extremely unlikely, as they were each committed to their own system.

9.20 Horton to write to the Heidelberg group to determine if they have successfully incorporated all curated structures from the literature into the SWEET2 database since CarbBank's demise (Minute 9.17: Action by Horton)
Horton reported that a BBA article by the Heidelberg group [Biochimica et Biophysica Acta 1760 (2006) 568–577] discusses the problems of incorporating structures from the literature into SWEET2 and how they have resolved these problems. Horton also gave a presentation on the carbohydrate databases that are currently available.

9.21 Biochemical compounds glossary. Cammack to co-opt a panel (Minute 12.1: Action by Cammack).
This was discussed under Item 5.1, the Chairman's report.

9.22 McNaught said that we should try to get synonym lists from Chemical Abstracts and Moss agreed to talk to them about this (Minute 12.2: Action by Moss).
This has been discussed with Sabine Kuhn from CAS and discussions will continue.

9.23 Tipton to distribute draft recommendations of glossary entries for the terms metabolomics vs. metabonomics for possible inclusion in a Newsletter (Minute 14.1: Action by Tipton)
Tipton reported that he had sent the definitions of these terms to Cammack for inclusion in the next Newsletter but a newsletter has not been published since.

9.24 Moss said that he could collate some of the examples of WHO's international non-proprietary names (INNs) that he has come across to provide to Berman, and that Berman and Apweiler were to investigate methodology once Moss has provided examples (Minute 10.1: Action by Moss, Berman and Apweiler)

Moss distributed some examples of INNs documents at the meeting. He said that, in the course of his work, he has to give a full name to antisense oligonucleotides and we have no documentation on how to name modified oligonucleotides. Moss reported that there is considerable interest in antisense oligonucleotides but some of them are very difficult to name as they could have up to twenty sets of brackets within a single name. Moss has talked to Sabine Kuhn and she will let him know how the naming problem is handled by CAS. Berman reported in her presentation that they are undergoing a remediation exercise and they also have the problem of naming antisense oligonucleotides. Moss reported that there are two separate problems: (1) Extending the one-letter code to include more complicated examples and (2) the actual naming of these compounds including those without a sugar unit. (**Action:** Sabine Kuhn to contact Moss about procedure used at CAS and Moss to contact Berman's associate regarding how PDB handle the problem of naming antisense oligonucleotides).

9.25 Schomburg reported that gene names rather than protein names are being used increasingly in papers and asked if we should issue a statement to discourage this practice. Cammack agreed to draft a Newsletter item regarding this (Minute 10.1: Action by Cammack)
No action yet taken.

9.26 Update of phosphorus document. Members were to provide McNaught with names of potential panel members and Dixon was to be consulted (Minutes 10.1 and 11.1: Action by all)
Dixon reported that he has been frustrated by the phosphorus document for years. He said that he had co-opted a panel to revise this document and that Berman has now agreed to join the panel. Dixon said that he was grateful to Moss and McNaught for the substantial contributions they have made to date. A draft will be ready within a few weeks but without the references. An application to be recognized as a project was sent to IUPAC and a decision by IUPAC will be made on May 19 2006. Members of the panel are Dixon, Moss, McNaught, Boyce, Berman, Dr. Larry Barnes of San Antonio, TX and Stephen B. Shears of the NIH.

9.27 Production of a new printed version of the Enzyme Nomenclature book. Vliegenthart said that if the IUBMB want a new version of the book to be published, then they should negotiate with different publishers and inform us of the decision they take. Cammack was to correspond with Azzi (Minute 9.18: Action by Cammack)
Cammack said that it might seem strange to be talking about a printed version of the Enzyme List when everything is available on the web. He said that some people prefer to consult a book rather than the web and that he still finds the 1992 version handy to have. Cammack provided a breakdown of the estimated page numbers for each section of a revised edition of the enzyme book. Tipton pointed out that it was possible to print out (or save as pdfs) the entire enzyme list or any selected parts of it from the MySQL database at
. A discussion on the pros and cons of publishing an updated version of the book met with considerable scepticism by the Committees. As a result, two options were put forward. The first was to drop the idea altogether and the second was for Schomburg to ask the IUBMB Executive (at the meeting in Kyoto in July 2006) for their opinion on the publication. It was agreed that we

would proceed with the second option (**Action:** Schomburg to consult with the IUBMB Executive)

9.28 Kazic suggested that we hold a workshop to determine if there is a community need for an increase in the activity of the Committees regarding the Enzyme List, which would require additional funds. Kazic and Tipton were to liaise regarding a workshop proposal to the NIH (Minute 8.8: Action by Kazic and Tipton)
Tipton has prepared a draft application for funding of a workshop and Kazic is to contact the NIH within the next month to get support for the proposal. The grant application must be submitted by August 2006.

9.29 Berman suggested that we apply to the Rockefeller Foundation to host the meeting at Bellagio, Lake Como in 2007. Berman to get information on Bellagio and to request references in support of application; Schomburg to make the application. (Minute 11.3; Action by Berman and Schomburg)
Schomburg reported that Berman's analysis had shown that such a meeting would be too expensive.

10. Funding Situation and Possibilities (Cammack, McNaught)

10.1 IUPAC
As discussed previously, IUPAC funding is available for projects on a competitive basis.

10.2 IUBMB
Our funding situation with regard to IUBMB is known ($15,000 over three years)

10.3 Other possibilities
As reported above (Item 5.1), Schomburg has applied to the Beilstein Foundation for funding for IUBMB activities in relation to enzyme classification. Ture Damhus said that he would be happy to approach his company on our behalf to see if they would be willing to fund activities such as our meetings. He said that we should contact him if we were interested in pursuing this. Apweiler reported that they get funding from companies for IUPHAR meetings (in the region of $15,000).

11. Future Projects and Activities

11.1 Update of the phosphorus document (Dixon)
This was discussed under Item 9.26. Dixon reported that there is a proposal to revise the book Principles of Chemical Nomenclature. The chapter on biochemical nomenclature is to be revised by Moss with assistance from Dixon. This project proposal is being submitted to IUPAC for approval.

11.2 Revision of carbohydrate nomenclature (Horton)
Horton reported that he will draft a small document on carbohydrates that is aimed particularly at biochemists. For revision of the main document, Horton requested input from members of the Committees (or outside) on the parts of the document that should be revised or additional items that should be added (**Action:** interested parties to submit suggestions to Horton regarding sections of the carbohydrate document that should be revised).

11.3 Publication of a new edition of the Enzyme Nomenclature book

Discussed under Item 9.27.

12. Newsletter

12.1 Publication of the 2006 Newsletter (Cammack)

Cammack said that this has not been done yet but that he would like to update it before distributing it to the Committees. Chemistry International might publish a newsletter and IUBMB Life would also publish a newsletter. Boyce suggested that items be added to a newsletter as they occur. Kazic suggested that we write an editorial but it was pointed out that these are not cited. Cammack informed the Committees that the Minutes of previous meetings have been published on the web. As some of the issues are sensitive, Schomburg will ask the Executive Committees to publish the Minutes in a condensed form in future. (**Action:** Boyce to collate items for a newsletter and Schomburg to consult with the Executive Committees about publishing a condensed version of the Minutes).

12.2 Items for the 2007 Newsletter

Discussed under Item 12.1

13. Any Other Business

There was no other business.

14. Date and Place of Meeting in 2007

It was agreed that the next meeting will be hosted by Horton in Bethesda, MD, on May 5-6, 2007.

15. Open Forum

15.1 Update on databases and related activities

Short presentations on updates to their databases and related activities were given by Apweiler, Berman, Kanehisa, Kazic, Moss and Schomburg.

Tipton asked Schomburg to approach the IUBMB about providing online access to the Journal Biochemistry and Molecular Biology Education (BAMBED) to members of the Committees (**Action:** Schomburg to make request to IUBMB for online access to BAMBED).

Ture Damhus said that he would be happy to help with any inorganic nomenclature, especially in connection with the phosphorus document and small molecules. He also reported that there is a section at the beginning of the new edition of the Red Book that describes all of the changes included in the new edition.

Moss reported that WHO produce INNs. They have included 158 enzymes and he needs to check that they have used the appropriate EC number. Moss said that he would prefer if they used the name of the protein rather than the name of the enzyme, which is an identifier for the reaction.

In relation to the Enzyme Database, Moss said that he had difficulties accessing the links to the GO ontology and that, since these added little value, they should be removed. However, following the conclusion of the meeting, several GO links were checked and shown to access the relevant information, so they will remain

in the Enzyme Database.

Dixon thanked Schomburg on behalf of the Committees for hosting the meeting.

---

8. Nomenclature Databases minute from the 2001 Minutes

8.1 The BioBabel project

By way of introduction, Cammack said that, over the years, Bairoch had wished to link the enzyme list to genetic databases and databases on nomenclature of organisms and to the scientific literature. He was pleased to say that Apweiler had good news on that front. Apweiler began with a short summary of the history of non-IUBMB-IUPHAR funding issues. In 1997, he had first obtained funding for enzyme nomenclature and classification through an EU grant and some funding from NSF. He said that Trinity College Dublin (TCD) received approximately $500,000 over five years for annotation purposes. This funding was about to run out, but he had secured new funding under a new EU project, which was due to start in August or September. This project has a total budget of 2,400,000 euros and will involve the EBI, the Swiss Institute of Bioinformatics (Bairoch's group), Michael Ashburner from the University of Cambridge, TCD and the BRENDA group in Köln. Berman said that this was a major step forward in terms of getting funding for this type of project. As noted by Purich, one has often to go to several places to get the information needed and to assemble this requires a large manpower input.
The title of the project is 'Enhanced Interoperability of Biological Databases by Standardization of Biochemical Terminology and Introduction of a Shared Ontology', or 'BioBabel'. The work packages all deal with standardization of nomenclature and terminology across the databases. A central work package (workpackage 5) involves the development and maintenance of shared biochemical terminology. This part of the project will take about ten man-years working on establishing the enzyme nomenclature database in Oracle and will incorporate the ENZYME database of Bairoch, the Enzyme List maintained by TCD, and the BRENDA database. Apweiler had been asked by IUPHAR to set up their receptor nomenclature database and this would integrate well with the enzyme database.

Apweiler said that these matters had been discussed at a meeting attended by a subcommittee of the Biochemical Nomenclature Committees (comprising, *inter alia*, Apweiler, Barrett, Boyce, Cammack, Dixon, Moss, Schomburg and Tipton) as the contract had to be finalised and returned to the European Commission. Cammack had been asked to respond on behalf of IUBMB on whether the Committees should take part in this contract. He agreed, but with the following provisos: (1) copyright remains with IUBMB, (2) there is a 2-month public review period as before and (3) the database would remain freely accessible to the biochemical community. If those conditions are met, it fulfilled the requirements from the Committees' side. (**Action:** Apweiler to provide details). Apweiler had also talked to Brian Clark in Virginia at the beginning of April. Clark said that he was pleased that these activities would be going on and he was supportive of them.

Cammack observed that there were basically two parts to this project, in relation to enzyme nomenclature: (1) creation of a database that would contain, amongst other things, a corrected version of the enzyme-list data that was already on Moss' website, and (2) creation of a mechanism that should assist the compilation of future enzyme entries. Boyce was creating entries that would be put in the database, so it was essential that she would have constant access to the database. Apweiler agreed and said that the database would be set up at EBI, but editorial control and intellectual property would stay unchanged. The only difference would be that, instead of new enzyme entries sitting on Boyce's computer, they would be in the Oracle database. The BioBabel proposal involved the creation of input and output technologies to allow

Boyce to annotate directly into the database. The procedures for assigning new EC numbers, and of making sure that only changes approved by the Committees were propagated, would remain unchanged.

Apweiler said that the principal person working on enzyme annotation was Boyce. Additional people on the project would be coming up with suggestions to her for improvements to the data. In due course, more data would be forwarded to the Biochemical Nomenclature Committees for approval. Apweiler hoped that this would improve the speed of assignment and avoid the departures from the normal approval procedure, whereby 2 months are allowed before an entry is made official, unless there is a request for further investigation.

In order for the system to operate effectively, there must be one master copy of the database; in other words, all additions and corrections are to be made to the database first, then transferred to other documents and databases. Apweiler needed a clear mandate that the database at the EBI would be the master database and asked the Committees to agree to this. Berman agreed that such a provision was essential. There was an analogous situation with the Protein Data Bank (PDB); funding and annotation is from many locations, but everybody inputs into one master copy. This is a principle that was established by the International Union of Crystallography (IUCR) a long time ago. Berman pointed out that, if in, say, five years time, there was a funding issue, the master copy would still be there, for the Committees to use as they thought fit.

McNaught asked for a written statement from Apweiler saying what was needed. Rolf reiterated that what he wants is, within the framework of BioBabel, to move the current flat files of the enzyme list into a relational database and to maintain the information there as the master copy of the data. The EBI would be the provider of the database and nothing else. All the material would stay in the public domain, copyright IUBMB. Apweiler said that nobody need see that the master copy was served out of the EBI. All the output would go to whatever URL or webpage we want to use, and run by whosoever the Committees designate.

There remained many inconsistencies in the current lists of enzymes, because although the various curators of each database had noted errors and corrected them in their own database, these had not been passed on to other databases. One person each from the EBI, from Geneva and from Köln would go through the data and list inconsistencies, which would then be passed to Boyce for correction, in consultation with others.

Tipton noted that, at that time, SWISS-PROT, which was updated periodically, was a year behind with the enzyme data supplied by the Committees and asked whether having the Oracle database system would rectify this situation. Apweiler replied that, as the database will be dealing with a controlled vocabulary, enzyme data would be directly incorporated into the corresponding tables of SWISS-PROT from the Oracle database. One of the other work packages deals with building a better dictionary of chemical compounds; Schomburg had already done quite a lot of work in this regard. Tipton pointed out that Kazic had also done a great deal of synonym work. He expressed the hope that the two groups would be able to collaborate on this and other aspects.

Cammack asked about the status of Moss' html database and said that, as he understood it, it was possible to output html files from Apweiler's database that can be put on Moss' website. He pointed out that the advantage of Moss' website was that it was relatively easy to add free text, diagrams and links to other databases that would not be handled easily by the Oracle database. Apweiler replied that, in their InterPro database, they can output as ASCII. He also said that you

can store data in whatever way you want and that it is only an output question. He said that modern databases have no problem handling graphic information.

Cammack asked if the setting up of this database would cause a delay in announcing new material, such as the “newenz” lists. Apweiler confirmed that until the database was functioning properly, the present system of creating entries would continue. Boyce should compile data and corrections while the database was being created. The only potential bottleneck would be during the initial upload of all data onto the database as the central master copy. Subsequently, all future updates would be handled through the master database. Berman asked Apweiler if he would have an executive summary of ‘what was going to be available and where’ so that database providers would be aware of what was available (**Action:** Apweiler).

Cammack asked Tipton, as the designated committee member responsible for the enzyme list, if he was content with the situation. Tipton replied that any decision had to be ratified by the IUBMB since they were the “owners” of the enzyme list. McNaught asked how long this arrangement would remain in place, and Apweiler replied that it would be for as long as there were funds to support it. McNaught said that there should be the opportunity to review the situation at intervals, possibly at Nomenclature Committee meetings, and this was agreed.

Cammack asked if the Committees were content to accept Apweiler’s proposals. This was agreed. McNaught recommended that, as the final decision rested with the IUBMB, the Committees should e-mail the IUBMB Executive Committee, explaining Apweiler’s requirements, saying what the Biochemical Nomenclature Committees have agreed to and get their confirmation that they are happy with such developments. Cammack asked if we needed to wait until the next meeting of the IUBMB but Tipton said that such a delay was unnecessary. (**Action:** Cammack).

APPENDIX III

IUPAC International Chemical Identifier (InChI)

Report to IUPAC Division VIII Committee, September 2006

1. New software release.

InChI version 1 software version 1.01 was released in August 2006.

It contains:

- InChI version 1 software version 1.01 documentation, and Windows and Linux (i386) executable programs
- InChI version 1 software version 1.01 source code and Application Program Interface (API)
- InChI validation protocol
- What's new in InChI software version 1.01

The release includes the following new features:

- InChI validation protocol to establish whether software that includes the InChI algorithm produces valid InChI
- InChI reversal: InChI to structure conversion (connection table, bond orders, charges, stereochemical parities; the resultant structures have no coordinates; success rate on average 99.7%)
- Several bug fixes that eliminate known InChI failures
- Some minor additional features

The InChI version in this package remains 1, not 1.01 because the chemical identifier produced remains same; only the software and documentation are updated.

2. *InChI development.*

Arrangements are in progress to provide additional resources at NIST, to facilitate further InChI development. We intend to establish a Guest Worker to work alongside Dmitrii Tchekhovskoi, with the following brief:

- To ensure that knowledge of the InChI protocol and software is shared with a second person

- To deconstruct the InChI software into an input and 'editing' module, a normaliser, a canonicaliser and a serialiser, for easier use by software developers

- To extend InChI to cover simple polymers, in accord with requirements specified at a meeting of the Task Group in Prague in June 2005

- To further explore the need for other InChI extensions and to implement in priority order as time permits

- To deal with any other requests for InChI enhancement as they arise

A likely candidate has been identified, and negotiations are in progress.

3. *InChI dissemination*

- Steve Heller has put together an extensive programme of formal presentations and talks with software developers, database providers and publishers, to ensure the continued effective spread of information about InChI, keeping up the pressure to take advantage of the facilities offered. Attached is a list of presentations (past and future) since the Beijing General Assembly.

- The facility to use Google to search for InChIs, temporarily disabled owing to changes in Google protocols, is now reinstated, but the characters 'InChI=' should now be omitted from the search string.

4. *InChI takeup*

- A list of software developers and database providers now using InChI is attached. Particularly noteworthy are PubChem's online 'InChI-generation-as-you-draw' facility ( ) and facilities for InChI-based similarity and substructure searching ( ).

- We are aware that there are other people/organizations making additions to InChI, such as Java add-ons/versions, etc. We may not hear about such activities until there is a problem or the work is finished. There is an irregular stream of questions and reports on the inchi-discuss listserver hosted at SourceForge.

- The Royal Society of Chemistry is working with groups at the Unilever Centre for Molecular Informatics (Cambridge) and Southampton University to develop publishing applications.

5. *InChI-related publications*

- The Chemical and Engineering News article noted as in press at the last meeting was published August 22 2005 (*C&EN*. vol.83, No.34, pp 39-40; web version at).

- An article on InChI will appear in *CI* November 2005 as part of the new 'Tools of the Trade' series.

- A selection of references to InChI-related articles is attached.

Alan McNaught
Steve Heller
30 August 2006

Presentations by Steve Heller since August 2005

The IUPAC InChI and Structural Changes in Chemical Information, Beilstein Institute, November 2005

Open Access/Open Source/Open Data and the IUPAC International Chemical Identifier (InChI), 1st German Conference on Chemoinformatics, Goslar, Germany, November 2005

Open Source/Open Access and the IUPAC International Chemical Identifier (InChI), 5th International Chemical Congress of Pacific Basin Societies - Pacifichem 2005 Conference, Honolulu, Hawaii, December 2005

What the IUPAC/NIST Chemical Identifier (InChI) Means to You, FDA Science Forum, Washington DC, April 2006

The Evolution and Revolution of Scientific Information Resources in the Last 50 Years, Prous Science - European Forum, Barcelona, Spain, September
2006

InChI takeup by software developers and database providers

Software:

1. Structure Drawing

a. ACD Labs: ChemSketch
b. CambridgeSoft: ChemDraw
c. ChemAxon: Marvin
d. BK-Chem:

2. Structure Search

a. IBM (internal project)

3. Analysis software

a. SciTegic:

4. Structure file interconversion

a. OpenBabel:

5. Other software

a. World Wide Molecular Matrix:

Databases:

1. NIST WebBook
2. NIH PubChem
3. NCI DTP
4. EPA - DSSTox
5. UC-SF ZINC project
6. KEGG
7. ISI Web of Science
8. Carcinogenic Potency
9. ChEBI
10. Wiley Mass Spectra
11. Prous Science Integrity
12. FDA GeneTox and Chronic/subchronic Databases
13. Compendium of Pesticide Common Names

Information resources:

B. Kosata:
P. Murray-Rust/N. Day:

Some articles and presentations that make use of InChI

- Chemical Structure Indexing of Toxicity Data on the Internet: Moving toward a Flat World, A. M. Richard, G. L. Swirsky, and M. C. Nicklaus, *Current Opinion in Drug Discovery and Development*, 2006, 9:314-325

- Bringing Chemical Data onto the Semantic Web, K. R. Taylor, R. J. Gledhill, J. W. Essex, J. G. Frey, S. W. Harris and D. C. De Roure, *J. Chem. Inf. Model*., 2006, **46**(3), 939-952. [ ]

- A Computer-Aided Drug Discovery System for Chemistry Teaching, Robert Gledhill, Sarah Kent, Brian Hudson, W. Graham Richards, Jonathan W. Essex, and Jeremy G. Frey, *J. Chem. Inf. Model.*, 2006, **46**(3), 960-970. [ ]

- , A. Monge, A. Arrault, C. Marot and L. Morin-Allory, presented at the *10th Electronic Computational Chemistry Conference,* April 2005

- Application of InChI to Curate, Index, and Query 3-D Structures, M.D. Prasanna, J. Vondrasek, A. Wlodawer and T.N. Bhat, *Proteins: Structure, Function, and Bioinformatics*, 2005, **60**, 1-4. [ ]

- Enhancement of the Chemical Semantic Web Through the Use of InChI Identifiers, S.J. Coles, N.E. Day, P. Murray-Rust, H.S. Rzepa and Y. Zhang, *Org. Biomol. Chem*., 2005, **3**(10), 1832-1834 [ ]

- Representation and Use of Chemistry in the Global Electronic Age, P. Murray-Rust, H.S. Rzepa, S.M. Tyrrell and Y. Zhang, *Org. Biomol. Chem.*, 2004, 3192-3203 [ ]

- P. Murray-Rust, H. S. Rzepa and Y. Zhang, , W3C Workshop on Semantic Web for Life Sciences, 27-28 October 2004, Cambridge, Massachusetts USA.

- P. Murray-Rust, H. S. Rzepa and S. Stein, , W3C Workshop on Semantic Web for Life Sciences, 27-28 October 2004, Cambridge, Massachusetts USA.

APPENDIX IV

Inorganic Preferred IUPAC Names (PINs) Meeting

Copenhagen, April 12-13, 2006

Present: Alan Hutton, Jan Reedijk, Jeff Leigh, Gerry Moss, Ebbe Nordlander, Ture Damhus, Alexander Senning (12 April only), Richard Hartshorn.

The aim of this meeting was to produce a detailed plan for work on PINs for inorganic and organometallic compounds not already covered by the new Blue Book. The key outcome was a plan for a project proposal for developing rules for assigning/choosing PINs for inorganic and organometallic compounds. Some suitable participants (core group and corresponding members) have been identified, and others will be approached. Several problematic areas have been identified and some progress has been made towards resolving those issues.

Notes on Agenda Items

1. Review of PINs concept and the way it is being implemented in the revised Blue Book (coverage, retained names, preselected names etc).

   Gerry Moss outlined the background to the PINs project. Essentially this revolved around the fact that users of nomenclature want "The IUPAC Name" for a compound or structure. There are several systematic ways of naming compounds and structures, all of which give unambiguous names and which are therefore satisfactory from a nomenclature point of view, as well as a number of trivial names that are still in wide use.

   Several years ago a meeting in Washington resolved that continued work on nomenclature should be a core activity for IUPAC and that there was a desire in the chemical community for there to be a single IUPAC name for a compound or structure. This led to the establishment of Division VIII when IUPAC Commissions were dissolved. This was consistent with the attempt to produce unique names for compounds (PINs) and that had been begun as part of the project to revise the Blue Book.

   A draft version of the Blue Book was posted on the internet for public review 2004-2005 and is currently undergoing further revision. Hard copy publication may well not be until 2007. Key features of the Blue Book are as follows:

   - *Wider coverage of organic nomenclature (compounds containing at least one carbon atom and only elements from Groups 13-17)*

- *All accepted unambiguous names are presented (general IUPAC nomenclature)*
- *One is identified as PIN*
- *Generally it involves substitutive nomenclature (with parent hydrides/structures)*
- *Trivial "retained" names (e.g. benzene, acetic acid, pyridine, acetone) are used as PINs where appropriate*
- *Some "retained" prefixes are used (e.g. tert-butyl, but not isopropyl) and Appendix 2 provides such prefixes and old names with PINs indicated*
- *"Preselected names" have been used where it was necessary to define an inorganic parent on which to base the PIN for an organic derivative – this does not mean that this preselected name need be chosen as the PIN for the inorganic parent (see sections P-10, P-11, and P-12)*
- *Retained names and prefixes and choice of larger substituent groups have normally been used for PINs so that the final name can be shorter.*

Discussion raised the question of whether the PIN for a compound is "forever", or should evolution be permitted. This may be a question for the Division Committee to consider.

2. Brief review of correspondence with Hervé Schepers (EU Taxation and Customs) in relation to end users and databases.

   Richard Hartshorn briefly reviewed the correspondence and introduced the ECICS database, which is likely to be useful when developing PINs. Key points are that PINs should wherever possible be short, simple, and already well known [subsequent note – permission has been obtained for the database to be circulated among the working group]

   A related comment was that deciphering names may become more important, particularly as obsolete names and non-PIN systematic names are used less. This may form the basis of a new project to provide a catalogue of obsolete names that have been used in the past for compounds and provide the modern equivalent/PIN [subsequent note – perhaps part of this would involve providing a series of pointers that identify the characteristics of different nomenclature systems as a way of recognising what sort of name is being used – a preliminary to deciphering a name]

3. Discussion of general principles: degree to which we make use of retained names; use of organic PINs within inorganic PINs (presumably yes/mostly); use of additive nomenclature (presumably yes/mostly); transient species, reaction intermediates, mixtures, phases, levels of characterisation and ill-defined structures (any link to INChIs?).

   This discussion flowed freely, but the following points were made:

- *Where organic fragments form part of an inorganic PIN, the organic PIN should be used wherever possible*
- *Additive nomenclature desirable for inorganic PINs*
- *More examples is better*
- *Principles of organic PINs may be important/useful (e.g. the PIN for H_3CSH may help in choosing the PIN for H_3SiSH)*
- *Wide use of additive and substitutive nomenclature*
- *Do not consider mixtures unless the individual compounds or structures are defined*
- *Phases and ill-defined compounds/structures should not be dealt with*
- *Compounds/structures can have more than one PIN (e.g. butan-2-ol – racemic, or R or S)*
- *PINs using compositional nomenclature may be required for materials of known composition but unknown structure*
- *Should different kinds of PINs be indicated in some way?(such as composition-based, structure-based)*

4. Specific issues related to use of additive nomenclature e.g. choice of central atom, mononuclear vs di/polynuclear. Any other issues?

An initial problem that will have to be addressed if additive nomenclature is to be used for inorganic PINs. This is tied to the fact that there is little guidance given regarding the choice of the central atom, which is an essential first step in developing a name using this kind of nomenclature. A series of rules need to be developed so that the same central atom(s) is(are) chosen by all users for the PIN. In the case of polynuclear species, more than one central atom can be used (and this often makes the name easier to construct), but alternatively, it may be possible to pick only one central atom and treat the remaining ones as ligands to the first. There was some discussion of this issue and the view was that it was likely that choosing multiple central atoms would be the best way forward. Probably this would mean all metal atoms, but there will also need to be consideration given to cases where elements from groups 13-17 are present (and which have often been treated as central atoms).

Should ligands themselves be named using additive or substitutive nomenclature? This may depend on the PINs that are chosen for the ligands.

Grammatical rules for the placement of κ/η symbols in complicated ligand names need to be more clearly defined.

Different classes of PINs may be required. For example some relatively common materials have well characterised (elemental) compositions even though the structure may not be known. This is an extension of the established idea that a molecule may have more than one PIN (e.g. where the structure is known but the configuration may not be). There may be five levels at which we consider providing PINs (composition, structure, isotopic substitution, configuration, conformation) and many of these are

already supported in the current organic PINs proposals. This then raises the question of whether the class of PIN should be indicated in some way. This may be an issue for the Division Committee to consider.

5. Identify sub-projects (based on classes of compounds? E.g. organometallic, coordination, main group) and define boundaries between them.

The first comment was that the flow diagram on p9 of the Red Book might help, as this directs the reader to appropriate nomenclature discussion for particular kinds of compounds. This effectively identifies sub-projects for PIN work.

The issues with selection of central atom and placement of κ/η symbols have to be resolved.

It was further noted that many of the coordination and organometallic compounds that are given in the Red Book may actually be rather straight-forward, as they already incorporate organic PINs (or at least they did to the best that could be done at the time). They will still be sub-projects, but perhaps not major ones.

Oxoacids and other main group compounds will need work, with particular attention being given to when retained names might be chosen as PINs, as opposed to systematic names. Some aspects of this task will be dependent on the outcome of the work on central atom choice.

6. Timescales – what can be done in parallel, what must be done sequentially?

Central atom selection needs to be clarified early in the process.
Oxoacids and main group probably represent the most challenging task and should be attempted next as it may require the most time and may identify other problems that will need to be sorted out.
Coordination compounds and organometallic compounds and placement of κ/η symbols should be able to be done later (and will depend on earlier sub-projects).

This is considered a large project with several interrelated parts. It may take three years or more (the related organic PINs project has been going for many years, albeit as part of a complete revision of the Blue Book). The working group envisaged annual meetings of those involved, to be held in association with the Division Committee meeting. There is likely to be a need for small sub-groups (2-3 people) to get together to address particular problems on an occasional basis. A first meeting might be able to be held in January – as a way of getting the project started sooner. Such a meeting would be in conjunction with a possible meeting of people involved in a revision of the Principles book (as there is a significant overlap of people between the two groups).

Catalogues and databases will provide useful material for testing and it is suggested that there should be reviews of the outcomes of the project by interested people throughout the process. Jan Reedijk indicated that he is in Brussels on a regular basis and might be able to liaise with Hervé Schepers as part of the review process.

7. Identify task group leaders and other participants for projects.

Richard Hartshorn will prepare the project proposal.
Ture Damhus, Alan Hutton, Ebbe Nordlander, and Jan Reedijk have indicated a willingness to participate in various parts of the project.

It was suggested that Andrey Yerin might be able to contribute, and that Karl-Heinz Hellwich be approached to see if there are any interested inorganic people at MDL.

Kevin Thurlow and Ole Norager might be approached for lists of relevant compounds

The rest of the meeting time was used to address the issue of central atom selection and what should be done in cases when there are multiple possible central atoms. No firm conclusions were drawn.

APPENDIX V

Nomenclature World Wide Web Database – Statistics

Statistics based on log of IP addresses used each day. Total usage to date about 5640000. Data on 202 countries recorded so far. Summary data for 1996-2005 at www.chem.qmul.ac.uk/iupac/usage/ For full details of each document see www.chem.qmul.ac.uk/iupac/ or

Average use **per week**

Year	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006
Total usage	296	650	1476	2786	5515	9813	15360	19105	20392	24617	32310
Search Facility	-	-	-	204	1663	4169	8355	11308	12192	15071	20641
Bibliographic Data	-	61	142	235	325	470	598	655	706	787	889
Map of Usage	-	7	8	29	37	58	83	78	107	131	229
IUPAC Nomenclature											
Class Names Glossary	138	157	430	693	1039	1504	2178	2492	2836	2944	3814
Physical Org Chem Glossary	29	36	136	343	751	1089	1796	1934	1782	1714	2359
Atomic Weight	23	48	95	144	310	651	964	1431	1525	1926	2247
Stereochemical Glossary	-	32	85	135	231	392	602	694	778	942	1252
Periodic Table	-	-	-	17	155	291	475	870	782	999	1063
Section F (Natural Products)	-	-	-	14	121	321	450	505	583	783	990
Medicinal Chemistry Glossary	-	-	56	87	150	316	532	601	636	708	830
Bioinorganic Glossary	-	-	61	108	201	391	633	570	523	664	815
Fused Ring	-	-	64	73	110	198	241	275	299	342	454
Numerical Term	-	18	27	35	54	99	150	189	238	325	404
Regular Organic Polymer	-	-	-	-	-	-	-	-	141	236	354
Ions and Radicals	-	-	-	-	72	150	196	226	245	278	353
Fullerenes	-	-	-	-	-	-	69	124	162	232	265
Phanes	-	-	31	42	56	80	95	135	181	209	243
Hantzsch Widman	12	14	31	46	56	89	116	125	154	195	226
Element Name > 100	-	-	-	20	45	78	87	93	147	170	226
Section H (Isotopic Label)	-	-	26	34	46	73	90	93	112	154	191
Spiro	-		-	26	47	90	114	115	137	163	180
von Baeyer	-	-	-	29	61	106	130	118	133	164	176
Delta Convention	8	9	19	30	54	82	110	106	121	130	157
Fullerene numbering	-	-	-	-	-	-	-	-	-	118	150
Lambda Convention	6	8	17	28	40	60	76	74	85	101	118
Phane II	-	-	-	-	-	-	-	59	68	86	95
Guide Errata	-	-	-	20	21	25	32	47	53	68	81
IUPAC/IUBMB Nomenclature											
Amino Acids & Peptides	31	62	135	186	359	670	1072	1366	1594	1918	2450
Carbohydrates	46	72	144	237	453	835	1156	1444	1266	1238	1561
Steroids	12	21	87	93	396	811	1213	1460	835	555	650
Vitamin B-6	-	-	-	34	95	155	267	466	306	302	466
Lipids	-	-	-	29	70	132	198	232	252	302	439

Tetrapyrroles	-	-	-	-	-	124	221	227	240	335	424
Vitamin D	-	-	-	-	47	69	125	209	385	348	401
Folic acid	-	-	-	60	58	210	208	304	284	293	385
Nucleic Acid Abbreviations	-	-	-	45	77	136	202	241	256	325	384
Glycoproteins	-	-	20	32	71	134	172	187	185	232	290
Tocopherol	-	-	21	33	48	80	150	274	232	260	279
Glycolipids	-	-	15	35	65	91	137	171	213	234	268
Lignans and Neolignans	-	-	-	-	-	71	123	137	170	237	264
Vitamin B-12	-	-	-	49	69	146	266	315	227	164	233
	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006
Carotenoids	-	-	-	-	46	84	128	148	167	199	231
Polypeptide Conformation	-	8	14	34	61	111	173	191	182	202	229
Cyclitols	-	-	21	51	72	113	174	178	177	207	216
Polynucleotide Conformation	-	7	15	27	44	68	92	103	124	164	189
Polysaccharide Conformation	-	8	14	26	49	82	134	153	155	162	174
Quinones with Isoprenoid Chain	-	-	-	-	-	47	90	105	116	162	169
Retinoids	-	-	-	-	35	71	99	126	140	136	155
Biochemical Phosphorus	-	-	-	-	62	103	151	147	133	139	152
Prenols	-	-	-	19	33	55	77	84	108	127	135
Polymerised Peptides	-	-	-	-	34	56	91	97	109	118	131
Both Biochemical Committees											
Committees' Homepage	18	38	65	123	268	423	653	801	1015	1218	1562
Newsletter	-	-	25	59	145	304	456	446	490	659	860
IUBMB Nomenclature											
Enzymes	16	54	124	320	1086	2088	3560	4260	5459	8837	12652
EC 1	-	-	-	35	241	487	922	1091	1497	2721	3996
EC 2	-	-	-	-	180	438	769	900	1242	2358	3490
EC 3	-	-	-	-	165	427	947	1054	1496	2333	3590
EC 3.4	16	54	>82	200	285	336	484	472	654	1117	1461
EC 4	-	-	-	-	90	223	410	423	635	1215	1623
EC 5	-	-	-	-	64	164	294	322	441	720	839
EC 6	-	-	-	-	46	138	239	261	374	674	819
reaction	-	-	-	-	48	119	381	650	1089	2295	3271
newenz	-	-	-	-	53	60	75	71	86	84	98
Enzyme Kinetics	-	-	16	61	152	249	365	441	547	687	963
Membrane Transport Proteins	-	-	-	-	-	-	93	157	188	287	337
Incomplete Nuc. Acid Sequence	-	9	20	31	50	75	103	137	205	293	332
Electron Transport Proteins	-	-	-	-	58	107	163	165	168	225	281
Biochemical Thermodynamics	-	-	22	40	66	107	132	148	170	224	283
Isoenzymes	-	-	14	28	68	106	124	123	135	159	191
Peptide Hormones	-	-	-	-	32	51	80	101	115	130	155
myo-inositol	-	-	11	23	43	74	125	125	113	139	138
Branched Chain Nucleic Acids	-	3	6	10	40	63	115	107	89	110	123
Multienzymes	-	-	10	13	18	25	37	36	43	52	58
Translation Factors	-	-	-	-	11	18	34	37	42	41	34